Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 04:36 PM EDT

PDB ID	:	13CY / pdb_000013cy
Title	:	Crystal structure of DUF190 bound to cAMP
Authors	:	Stockbridge, R.B.; Peralta, C.M.
Deposited on	:	2026-04-30
Resolution	:	1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

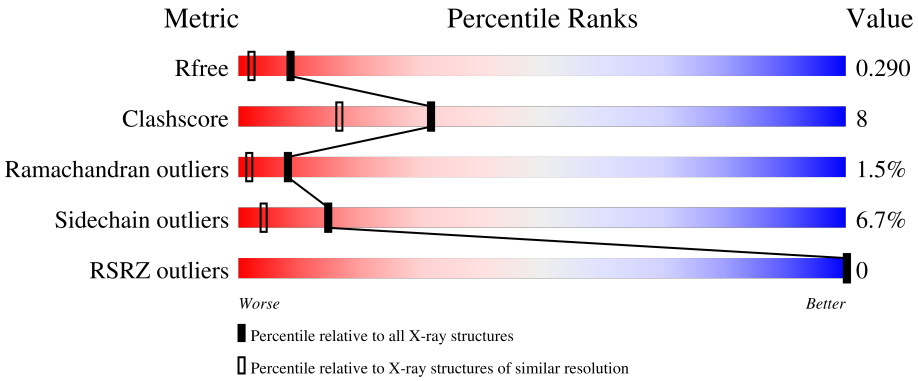
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	61% 20% 6% 14%
1	B	122	65% 22% • 11%
1	C	122	66% 16% 18%
1	D	122	70% 11% • 17%
1	E	122	57% 27% • 16%

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Mol	Chain	Length	Quality of chain
1	F	122	66% 16% 6% 12%
1	G	122	58% 26% 16%
1	H	122	64% 19% 13%
1	I	122	66% 14% 18%
1	J	122	66% 15% 18%
1	K	122	61% 21% 17%
1	L	122	70% 15% 11%
1	M	122	65% 15% 18%
1	N	122	58% 25% 17%
1	O	122	66% 19% 13%
1	P	122	69% 11% 18%
1	Q	122	69% 15% 16%
1	R	122	69% 19% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CMP	D	201[A]	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15143 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DUF190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	101	Total	C	N	O	S	0	1	0
			796	505	135	152	4			
1	E	103	Total	C	N	O	S	0	0	0
			804	513	136	151	4			
1	F	107	Total	C	N	O	S	0	3	0
			861	551	145	161	4			
1	C	100	Total	C	N	O	S	0	0	0
			776	493	133	146	4			
1	A	105	Total	C	N	O	S	0	0	0
			828	531	138	155	4			
1	B	108	Total	C	N	O	S	0	0	0
			849	544	145	156	4			
1	I	100	Total	C	N	O	S	0	0	0
			776	492	132	148	4			
1	G	103	Total	C	N	O	S	0	0	0
			804	513	136	151	4			
1	H	106	Total	C	N	O	S	0	1	0
			844	540	142	158	4			
1	J	100	Total	C	N	O	S	0	1	0
			781	495	132	150	4			
1	K	101	Total	C	N	O	S	0	0	0
			788	501	134	149	4			
1	L	108	Total	C	N	O	S	0	2	0
			859	549	144	162	4			
1	M	100	Total	C	N	O	S	0	1	0
			779	496	133	146	4			
1	N	101	Total	C	N	O	S	0	0	0
			781	496	133	149	3			
1	O	106	Total	C	N	O	S	0	0	0
			833	534	139	156	4			
1	P	100	Total	C	N	O	S	0	2	0
			790	501	133	152	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	102	Total	C	N	O	S	0	0	0
			784	499	132	150	3			
1	R	108	Total	C	N	O	S	0	1	0
			858	549	145	160	4			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	116	GLY	-	expression tag	UNP A0A1W1WVA9
D	117	GLY	-	expression tag	UNP A0A1W1WVA9
D	118	SER	-	expression tag	UNP A0A1W1WVA9
D	119	LEU	-	expression tag	UNP A0A1W1WVA9
D	120	VAL	-	expression tag	UNP A0A1W1WVA9
D	121	PRO	-	expression tag	UNP A0A1W1WVA9
D	122	ARG	-	expression tag	UNP A0A1W1WVA9
E	116	GLY	-	expression tag	UNP A0A1W1WVA9
E	117	GLY	-	expression tag	UNP A0A1W1WVA9
E	118	SER	-	expression tag	UNP A0A1W1WVA9
E	119	LEU	-	expression tag	UNP A0A1W1WVA9
E	120	VAL	-	expression tag	UNP A0A1W1WVA9
E	121	PRO	-	expression tag	UNP A0A1W1WVA9
E	122	ARG	-	expression tag	UNP A0A1W1WVA9
F	116	GLY	-	expression tag	UNP A0A1W1WVA9
F	117	GLY	-	expression tag	UNP A0A1W1WVA9
F	118	SER	-	expression tag	UNP A0A1W1WVA9
F	119	LEU	-	expression tag	UNP A0A1W1WVA9
F	120	VAL	-	expression tag	UNP A0A1W1WVA9
F	121	PRO	-	expression tag	UNP A0A1W1WVA9
F	122	ARG	-	expression tag	UNP A0A1W1WVA9
C	116	GLY	-	expression tag	UNP A0A1W1WVA9
C	117	GLY	-	expression tag	UNP A0A1W1WVA9
C	118	SER	-	expression tag	UNP A0A1W1WVA9
C	119	LEU	-	expression tag	UNP A0A1W1WVA9
C	120	VAL	-	expression tag	UNP A0A1W1WVA9
C	121	PRO	-	expression tag	UNP A0A1W1WVA9
C	122	ARG	-	expression tag	UNP A0A1W1WVA9
A	116	GLY	-	expression tag	UNP A0A1W1WVA9
A	117	GLY	-	expression tag	UNP A0A1W1WVA9
A	118	SER	-	expression tag	UNP A0A1W1WVA9
A	119	LEU	-	expression tag	UNP A0A1W1WVA9
A	120	VAL	-	expression tag	UNP A0A1W1WVA9
A	121	PRO	-	expression tag	UNP A0A1W1WVA9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ARG	-	expression tag	UNP A0A1W1WVA9
B	116	GLY	-	expression tag	UNP A0A1W1WVA9
B	117	GLY	-	expression tag	UNP A0A1W1WVA9
B	118	SER	-	expression tag	UNP A0A1W1WVA9
B	119	LEU	-	expression tag	UNP A0A1W1WVA9
B	120	VAL	-	expression tag	UNP A0A1W1WVA9
B	121	PRO	-	expression tag	UNP A0A1W1WVA9
B	122	ARG	-	expression tag	UNP A0A1W1WVA9
I	116	GLY	-	expression tag	UNP A0A1W1WVA9
I	117	GLY	-	expression tag	UNP A0A1W1WVA9
I	118	SER	-	expression tag	UNP A0A1W1WVA9
I	119	LEU	-	expression tag	UNP A0A1W1WVA9
I	120	VAL	-	expression tag	UNP A0A1W1WVA9
I	121	PRO	-	expression tag	UNP A0A1W1WVA9
I	122	ARG	-	expression tag	UNP A0A1W1WVA9
G	116	GLY	-	expression tag	UNP A0A1W1WVA9
G	117	GLY	-	expression tag	UNP A0A1W1WVA9
G	118	SER	-	expression tag	UNP A0A1W1WVA9
G	119	LEU	-	expression tag	UNP A0A1W1WVA9
G	120	VAL	-	expression tag	UNP A0A1W1WVA9
G	121	PRO	-	expression tag	UNP A0A1W1WVA9
G	122	ARG	-	expression tag	UNP A0A1W1WVA9
H	116	GLY	-	expression tag	UNP A0A1W1WVA9
H	117	GLY	-	expression tag	UNP A0A1W1WVA9
H	118	SER	-	expression tag	UNP A0A1W1WVA9
H	119	LEU	-	expression tag	UNP A0A1W1WVA9
H	120	VAL	-	expression tag	UNP A0A1W1WVA9
H	121	PRO	-	expression tag	UNP A0A1W1WVA9
H	122	ARG	-	expression tag	UNP A0A1W1WVA9
J	116	GLY	-	expression tag	UNP A0A1W1WVA9
J	117	GLY	-	expression tag	UNP A0A1W1WVA9
J	118	SER	-	expression tag	UNP A0A1W1WVA9
J	119	LEU	-	expression tag	UNP A0A1W1WVA9
J	120	VAL	-	expression tag	UNP A0A1W1WVA9
J	121	PRO	-	expression tag	UNP A0A1W1WVA9
J	122	ARG	-	expression tag	UNP A0A1W1WVA9
K	116	GLY	-	expression tag	UNP A0A1W1WVA9
K	117	GLY	-	expression tag	UNP A0A1W1WVA9
K	118	SER	-	expression tag	UNP A0A1W1WVA9
K	119	LEU	-	expression tag	UNP A0A1W1WVA9
K	120	VAL	-	expression tag	UNP A0A1W1WVA9
K	121	PRO	-	expression tag	UNP A0A1W1WVA9

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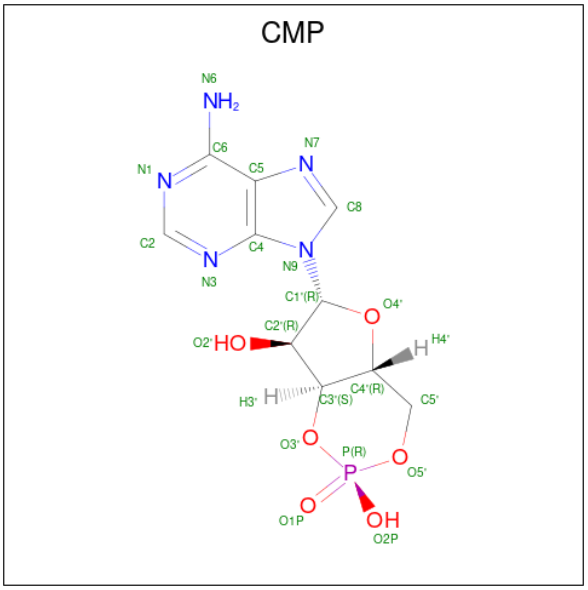
Chain	Residue	Modelled	Actual	Comment	Reference
K	122	ARG	-	expression tag	UNP A0A1W1WVA9
L	116	GLY	-	expression tag	UNP A0A1W1WVA9
L	117	GLY	-	expression tag	UNP A0A1W1WVA9
L	118	SER	-	expression tag	UNP A0A1W1WVA9
L	119	LEU	-	expression tag	UNP A0A1W1WVA9
L	120	VAL	-	expression tag	UNP A0A1W1WVA9
L	121	PRO	-	expression tag	UNP A0A1W1WVA9
L	122	ARG	-	expression tag	UNP A0A1W1WVA9
M	116	GLY	-	expression tag	UNP A0A1W1WVA9
M	117	GLY	-	expression tag	UNP A0A1W1WVA9
M	118	SER	-	expression tag	UNP A0A1W1WVA9
M	119	LEU	-	expression tag	UNP A0A1W1WVA9
M	120	VAL	-	expression tag	UNP A0A1W1WVA9
M	121	PRO	-	expression tag	UNP A0A1W1WVA9
M	122	ARG	-	expression tag	UNP A0A1W1WVA9
N	116	GLY	-	expression tag	UNP A0A1W1WVA9
N	117	GLY	-	expression tag	UNP A0A1W1WVA9
N	118	SER	-	expression tag	UNP A0A1W1WVA9
N	119	LEU	-	expression tag	UNP A0A1W1WVA9
N	120	VAL	-	expression tag	UNP A0A1W1WVA9
N	121	PRO	-	expression tag	UNP A0A1W1WVA9
N	122	ARG	-	expression tag	UNP A0A1W1WVA9
O	116	GLY	-	expression tag	UNP A0A1W1WVA9
O	117	GLY	-	expression tag	UNP A0A1W1WVA9
O	118	SER	-	expression tag	UNP A0A1W1WVA9
O	119	LEU	-	expression tag	UNP A0A1W1WVA9
O	120	VAL	-	expression tag	UNP A0A1W1WVA9
O	121	PRO	-	expression tag	UNP A0A1W1WVA9
O	122	ARG	-	expression tag	UNP A0A1W1WVA9
P	116	GLY	-	expression tag	UNP A0A1W1WVA9
P	117	GLY	-	expression tag	UNP A0A1W1WVA9
P	118	SER	-	expression tag	UNP A0A1W1WVA9
P	119	LEU	-	expression tag	UNP A0A1W1WVA9
P	120	VAL	-	expression tag	UNP A0A1W1WVA9
P	121	PRO	-	expression tag	UNP A0A1W1WVA9
P	122	ARG	-	expression tag	UNP A0A1W1WVA9
Q	116	GLY	-	expression tag	UNP A0A1W1WVA9
Q	117	GLY	-	expression tag	UNP A0A1W1WVA9
Q	118	SER	-	expression tag	UNP A0A1W1WVA9
Q	119	LEU	-	expression tag	UNP A0A1W1WVA9
Q	120	VAL	-	expression tag	UNP A0A1W1WVA9
Q	121	PRO	-	expression tag	UNP A0A1W1WVA9

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	122	ARG	-	expression tag	UNP A0A1W1WVA9
R	116	GLY	-	expression tag	UNP A0A1W1WVA9
R	117	GLY	-	expression tag	UNP A0A1W1WVA9
R	118	SER	-	expression tag	UNP A0A1W1WVA9
R	119	LEU	-	expression tag	UNP A0A1W1WVA9
R	120	VAL	-	expression tag	UNP A0A1W1WVA9
R	121	PRO	-	expression tag	UNP A0A1W1WVA9
R	122	ARG	-	expression tag	UNP A0A1W1WVA9

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	1
			44	20	10	12	2		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	F	1	Total	C	N	O	P	0	1
			44	20	10	12	2		
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	I	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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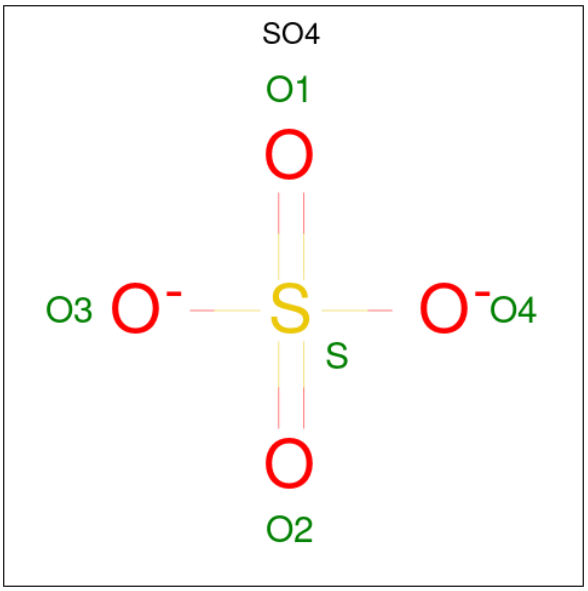
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	H	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	J	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	L	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	L	1	Total	C	N	O	P	0	1
			44	20	10	12	2		
2	M	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	O	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	O	1	Total	C	N	O	P	0	1
			44	20	10	12	2		
2	Q	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	R	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	R	1	Total	C	N	O	P	0	1
			44	20	10	12	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	P	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0
5	F	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	I	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0
5	R	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DUF190

Chain D:

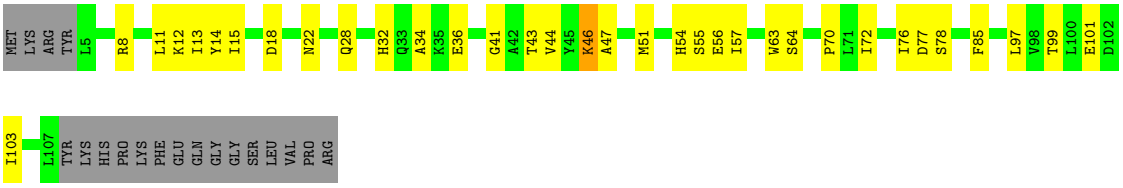




• Molecule 1: DUF190

Chain E:

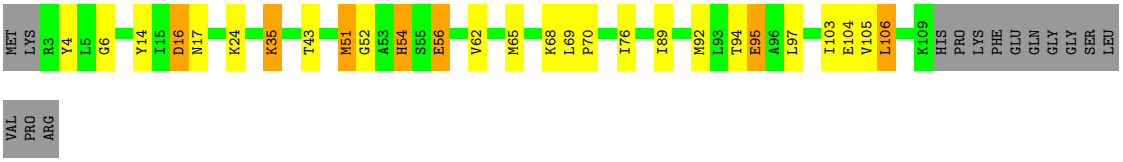




• Molecule 1: DUF190

Chain F:





• Molecule 1: DUF190

Chain C:

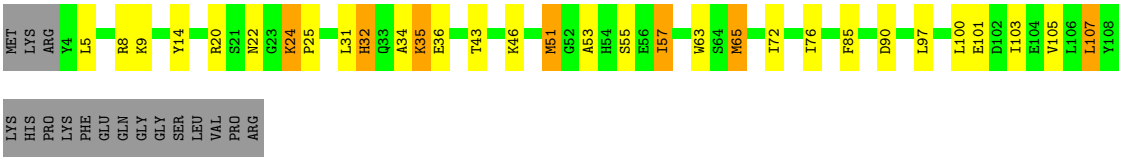




• Molecule 1: DUF190

Chain A:

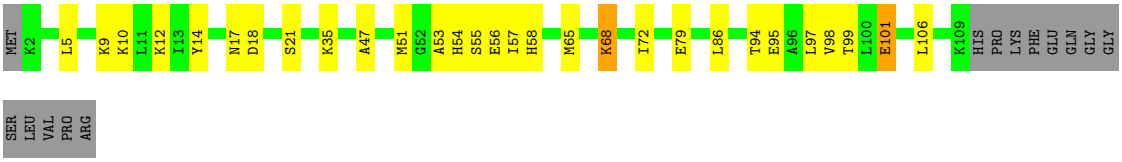




• Molecule 1: DUF190

Chain B:

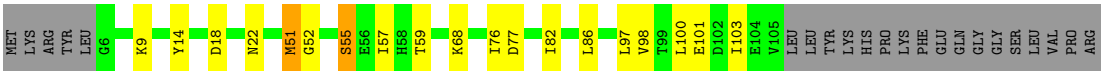




• Molecule 1: DUF190

Chain I:





• Molecule 1: DUF190

Chain G:

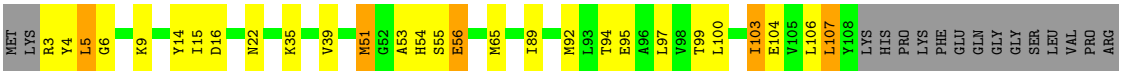




• Molecule 1: DUF190

Chain H:





• Molecule 1: DUF190

Chain J:

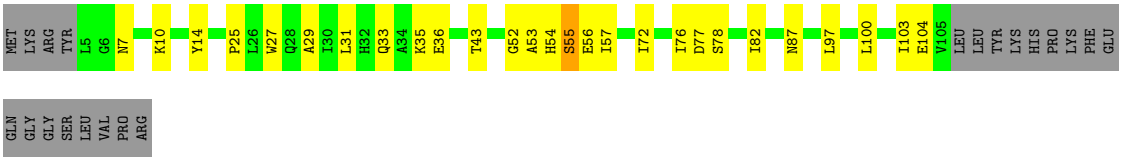




• Molecule 1: DUF190

Chain K:





• Molecule 1: DUF190

Chain L:





• Molecule 1: DUF190

Chain M:





• Molecule 1: DUF190

Chain N:





• Molecule 1: DUF190

Chain O:





• Molecule 1: DUF190

Chain P:

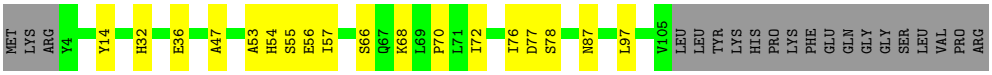




• Molecule 1: DUF190

Chain Q:

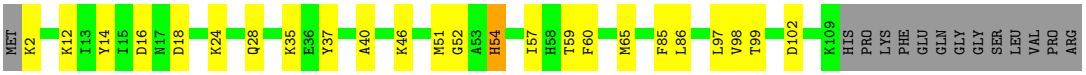




• Molecule 1: DUF190

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.96Å 75.11Å 235.76Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	56.95 – 1.94 56.95 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (56.95-1.94) 99.5 (56.95-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.94Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.283 , 0.290 0.283 , 0.290	Depositor DCC
R_{free} test set	6567 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.439 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.438 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.437 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.418 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.440 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15143	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CMP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.12	0/843	0.40	1/1138 (0.1%)
1	B	0.14	0/864	0.35	0/1165
1	C	0.12	0/789	0.30	0/1064
1	D	0.14	0/809	0.30	0/1091
1	E	0.11	0/817	0.34	0/1102
1	F	0.16	0/886	0.39	0/1196
1	G	0.11	0/817	0.32	0/1102
1	H	0.12	0/862	0.35	0/1163
1	I	0.13	0/789	0.31	0/1065
1	J	0.14	0/797	0.35	0/1076
1	K	0.12	0/801	0.36	0/1080
1	L	0.13	0/880	0.35	0/1188
1	M	0.12	0/795	0.31	0/1072
1	N	0.10	0/794	0.30	0/1073
1	O	0.12	0/848	0.32	0/1145
1	P	0.14	0/809	0.34	0/1091
1	Q	0.11	0/797	0.34	0/1077
1	R	0.11	0/876	0.33	0/1181
All	All	0.13	0/14873	0.34	1/20069 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	ASN	CB-CA-C	-6.29	108.68	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	837	17	0
1	B	849	0	861	19	0
1	C	776	0	782	10	0
1	D	796	0	800	15	0
1	E	804	0	819	21	0
1	F	861	0	867	18	0
1	G	804	0	819	21	0
1	H	844	0	854	17	0
1	I	776	0	775	11	0
1	J	781	0	779	8	0
1	K	788	0	797	20	0
1	L	859	0	862	14	0
1	M	779	0	786	12	0
1	N	781	0	779	15	0
1	O	833	0	839	12	0
1	P	790	0	794	8	0
1	Q	784	0	781	10	0
1	R	858	0	869	14	0
2	A	22	0	11	1	0
2	B	44	0	22	3	0
2	D	44	0	22	8	0
2	E	22	0	11	1	0
2	F	44	0	22	5	0
2	G	22	0	11	2	0
2	H	22	0	11	1	0
2	I	22	0	11	2	0
2	J	22	0	11	1	0
2	L	66	0	33	5	0
2	M	22	0	11	1	0
2	O	66	0	33	5	0
2	Q	22	0	11	2	0
2	R	66	0	33	6	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	K	1	0	0	0	0
3	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1	0	0	0	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	5	0	0	0	0
4	O	5	0	0	1	0
4	R	5	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	R	2	0	0	1	0
All	All	15143	0	14953	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:202[A]:CMP:H2	2:R:202[A]:CMP:C2	0.97	1.50
2:A:201:CMP:C2	2:A:201:CMP:H2	0.97	1.50
2:L:202[A]:CMP:C2	2:L:202[A]:CMP:H2	0.97	1.50
2:O:202[A]:CMP:C2	2:O:202[A]:CMP:H2	0.97	1.50
2:M:201:CMP:C2	2:M:201:CMP:H2	0.97	1.49
2:O:202[B]:CMP:H2	2:O:202[B]:CMP:C2	0.97	1.49
2:G:201:CMP:H2	2:G:201:CMP:C2	0.97	1.49
2:D:201[B]:CMP:H2	2:D:201[B]:CMP:C2	0.97	1.49
2:E:201:CMP:H2	2:E:201:CMP:C2	0.97	1.49
2:I:201:CMP:H2	2:I:201:CMP:C2	0.97	1.49
2:O:201:CMP:C2	2:O:201:CMP:H2	0.97	1.48
2:D:201[A]:CMP:C2	2:D:201[A]:CMP:H2	0.97	1.48
2:L:202[B]:CMP:H2	2:L:202[B]:CMP:C2	0.97	1.48
2:R:201:CMP:C2	2:R:201:CMP:H2	0.97	1.48
2:B:202:CMP:C2	2:B:202:CMP:H2	0.97	1.48
2:F:201[A]:CMP:C2	2:F:201[A]:CMP:H2	0.97	1.48
2:L:201:CMP:H2	2:L:201:CMP:C2	0.97	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:CMP:H2	2:B:201:CMP:C2	0.97	1.47
2:H:201:CMP:C2	2:H:201:CMP:H2	0.97	1.47
2:R:202[B]:CMP:H2	2:R:202[B]:CMP:C2	0.97	1.47
2:F:201[B]:CMP:H2	2:F:201[B]:CMP:C2	0.97	1.47
2:J:201:CMP:C2	2:J:201:CMP:H2	0.97	1.47
2:Q:201:CMP:H2	2:Q:201:CMP:C2	0.97	1.47
2:D:201[A]:CMP:HN62	1:F:76:ILE:H	1.26	0.84
1:K:35:LYS:NZ	1:L:55:SER:O	2.14	0.81
1:K:76:ILE:H	2:L:202[B]:CMP:HN62	1.29	0.80
1:D:51:MET:HE1	1:F:35:LYS:HG2	1.67	0.77
1:D:51:MET:HE3	1:D:57:ILE:HG13	1.69	0.74
1:E:47:ALA:HB3	1:E:70:PRO:HG2	1.71	0.73
1:A:35:LYS:NZ	1:B:54:HIS:O	2.22	0.73
1:J:101:GLU:HB3	1:L:103:ILE:HG22	1.71	0.73
1:Q:47:ALA:HB3	1:Q:70:PRO:HG2	1.72	0.71
1:O:79:GLU:OE2	1:O:83:ARG:NH1	2.24	0.70
1:D:20:ARG:HH12	1:A:65:MET:HB3	1.56	0.69
1:D:103:ILE:HG22	1:E:101:GLU:HB3	1.77	0.67
1:L:4:TYR:O	1:L:5:LEU:HB2	1.93	0.67
1:G:47:ALA:HB3	1:G:70:PRO:HG2	1.78	0.66
1:Q:76:ILE:H	2:R:202[B]:CMP:HN62	1.43	0.65
1:O:14:TYR:HB2	1:O:97:LEU:HB3	1.78	0.64
1:F:14:TYR:HB2	1:F:97:LEU:HB3	1.79	0.63
1:H:14:TYR:HB2	1:H:97:LEU:HB3	1.81	0.62
1:B:14:TYR:HB2	1:B:97:LEU:HB3	1.80	0.62
1:I:51:MET:HE3	1:I:57:ILE:HG12	1.81	0.62
1:Q:54:HIS:O	1:Q:56:GLU:N	2.32	0.62
1:D:9:LYS:HB3	1:D:100:LEU:HD11	1.81	0.61
1:K:103:ILE:HD12	1:L:99:THR:HB	1.83	0.61
1:F:89:ILE:HB	1:F:92:MET:HE2	1.83	0.60
1:I:52:GLY:O	1:I:55:SER:OG	2.19	0.60
1:A:43:THR:OG1	2:B:202:CMP:H8	2.03	0.59
1:Q:77:ASP:OD1	1:Q:78:SER:N	2.35	0.59
1:F:51:MET:O	2:F:201[B]:CMP:H5'1	2.02	0.59
1:L:89:ILE:HB	1:L:92:MET:HE2	1.85	0.58
1:L:14:TYR:HB2	1:L:97:LEU:HB3	1.84	0.58
1:F:4:TYR:CE2	1:F:6:GLY:HA2	2.38	0.58
1:K:36:GLU:OE1	1:O:7:ASN:ND2	2.37	0.58
1:M:52:GLY:HA2	1:O:41:GLY:HA3	1.85	0.58
1:H:5:LEU:HD13	1:H:6:GLY:H	1.67	0.58
1:C:9:LYS:HB3	1:C:100:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:LYS:N	5:R:302:HOH:O	2.37	0.57
1:B:9:LYS:HE3	1:B:79:GLU:HG3	1.86	0.57
1:R:51:MET:HE2	1:R:57:ILE:HG12	1.87	0.56
1:I:51:MET:HE1	1:H:35:LYS:HG2	1.88	0.56
1:J:52:GLY:HA2	1:L:41:GLY:HA3	1.86	0.56
1:D:51:MET:HE3	1:D:57:ILE:CG1	2.35	0.55
1:E:77:ASP:OD1	1:E:78:SER:N	2.37	0.55
1:E:18:ASP:OD1	1:E:18:ASP:N	2.34	0.55
1:I:101:GLU:HB3	1:H:103:ILE:HG22	1.89	0.55
1:D:6:GLY:N	5:D:301:HOH:O	2.40	0.55
1:L:3:ARG:HG2	1:L:5:LEU:HD13	1.90	0.53
1:A:14:TYR:HB2	1:A:97:LEU:HB3	1.90	0.53
1:A:35:LYS:HE2	1:B:51:MET:HE2	1.92	0.52
1:D:51:MET:C	2:D:201[A]:CMP:H5'1	2.34	0.52
1:C:52:GLY:O	1:C:55:SER:OG	2.21	0.52
1:A:107:LEU:HD22	1:B:97:LEU:HD13	1.91	0.52
1:I:86:LEU:HD11	1:I:98:VAL:HG11	1.92	0.51
1:C:14:TYR:HB2	1:C:97:LEU:HB3	1.91	0.51
1:N:20:ARG:NH1	1:N:23:GLY:O	2.43	0.51
1:G:74:GLU:OE2	1:H:14:TYR:OH	2.20	0.51
1:N:14:TYR:CD2	1:N:72:ILE:HD12	2.46	0.51
1:G:40:ALA:O	1:H:53:ALA:N	2.43	0.51
1:G:51:MET:HE2	1:G:55:SER:HA	1.92	0.51
1:K:87:ASN:HB3	1:Q:87:ASN:HB3	1.92	0.51
1:P:48:ALA:HB2	1:R:46:LYS:HG3	1.93	0.51
1:N:29:ALA:O	1:N:33:GLN:HG2	2.11	0.51
1:Q:14:TYR:CD2	1:Q:72:ILE:HD12	2.47	0.50
1:O:70:PRO:HG3	2:O:202[B]:CMP:H5'1	1.93	0.50
1:E:14:TYR:CD2	1:E:72:ILE:HD12	2.47	0.50
1:A:14:TYR:CD2	1:A:72:ILE:HD12	2.46	0.50
1:H:35:LYS:NZ	1:H:39:VAL:O	2.42	0.50
1:B:94:THR:OG1	1:B:95:GLU:N	2.45	0.50
1:C:51:MET:SD	1:B:35:LYS:HE3	2.52	0.50
1:M:58:HIS:HB3	1:M:68:LYS:O	2.12	0.50
1:G:32:HIS:O	1:G:36:GLU:HG2	2.12	0.50
1:R:86:LEU:HD21	1:R:98:VAL:HG11	1.93	0.50
1:E:34:ALA:HA	1:E:85:PHE:HE2	1.77	0.50
1:A:32:HIS:O	1:A:36:GLU:HG2	2.12	0.50
1:M:103:ILE:HG22	1:N:101:GLU:HB3	1.94	0.50
1:O:94:THR:OG1	1:O:95:GLU:N	2.40	0.50
1:H:3:ARG:HA	1:H:107:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:ASP:OD1	1:J:78:SER:N	2.39	0.49
1:O:51:MET:HE2	1:O:57:ILE:HG12	1.94	0.49
1:E:32:HIS:O	1:E:36:GLU:HG2	2.13	0.48
1:K:14:TYR:CD2	1:K:72:ILE:HD12	2.48	0.48
1:G:9:LYS:HD2	1:G:100:LEU:HD22	1.96	0.48
1:J:76:ILE:HG23	1:J:103:ILE:HD11	1.95	0.48
1:J:35:LYS:NZ	1:K:52:GLY:O	2.47	0.48
1:B:65:MET:HE3	1:B:65:MET:O	2.14	0.48
1:L:51:MET:HE2	1:L:57:ILE:HG12	1.95	0.48
1:C:35:LYS:NZ	1:C:39:VAL:O	2.36	0.47
1:R:14:TYR:HB2	1:R:97:LEU:HB3	1.95	0.47
1:G:37:TYR:OH	1:N:37:TYR:OH	2.32	0.47
1:D:18[B]:ASP:OD1	1:D:19:ASP:N	2.47	0.47
1:J:58:HIS:HB3	1:J:68:LYS:O	2.14	0.47
1:G:87:ASN:HB3	1:N:87:ASN:HB3	1.94	0.47
1:M:53:ALA:N	1:O:40:ALA:O	2.33	0.47
1:K:14:TYR:HB2	1:K:97:LEU:HB3	1.96	0.47
2:I:201:CMP:O1P	1:G:58:HIS:ND1	2.48	0.47
1:G:13:ILE:HG22	1:G:15:ILE:HG23	1.96	0.47
1:D:97:LEU:HD22	2:D:201[A]:CMP:C4	2.50	0.46
1:P:53:ALA:N	1:R:40:ALA:O	2.34	0.46
1:C:57:ILE:HG22	1:C:59:THR:HG23	1.98	0.46
1:K:25:PRO:HB2	1:K:27:TRP:CD1	2.51	0.46
1:P:58:HIS:HB3	1:P:68:LYS:O	2.15	0.46
1:D:20:ARG:HH12	1:A:65:MET:CB	2.26	0.46
1:E:57:ILE:HG21	1:A:63:TRP:HH2	1.81	0.46
1:C:103:ILE:HG22	1:A:101:GLU:HG2	1.97	0.46
1:B:68:LYS:HB3	1:B:68:LYS:HE2	1.69	0.46
1:K:43:THR:OG1	2:L:202[B]:CMP:N7	2.48	0.46
1:G:104:GLU:O	1:H:99:THR:HA	2.16	0.46
1:M:51:MET:HE1	1:O:35:LYS:HG2	1.98	0.46
1:A:51:MET:HE2	1:A:55:SER:HA	1.98	0.45
1:H:65:MET:HA	1:H:65:MET:HE3	1.98	0.45
1:N:9:LYS:HD2	1:N:100:LEU:HG	1.97	0.45
1:A:9:LYS:HE3	1:A:100:LEU:HD22	1.97	0.45
1:L:65:MET:HE3	1:L:65:MET:HB3	1.75	0.45
1:F:4:TYR:C	1:F:6:GLY:H	2.24	0.45
1:C:16:ASP:OD2	1:C:68:LYS:NZ	2.49	0.45
1:R:51:MET:HG3	1:R:52:GLY:H	1.82	0.45
1:E:14:TYR:HB2	1:E:97:LEU:HB3	1.98	0.45
1:E:34:ALA:HA	1:E:85:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LYS:HE2	1:B:35:LYS:HA	1.99	0.45
1:I:14:TYR:HB2	1:I:97:LEU:HB3	1.98	0.45
1:I:76:ILE:HG23	1:I:103:ILE:HD11	1.98	0.45
1:P:51:MET:HE1	1:R:35:LYS:HG2	1.97	0.45
1:B:47:ALA:HB2	1:B:72:ILE:HD11	1.99	0.45
1:K:29:ALA:O	1:K:33:GLN:HG2	2.16	0.45
1:M:77:ASP:HB3	1:M:82:ILE:HG12	1.98	0.45
1:Q:32:HIS:O	1:Q:36:GLU:HG2	2.17	0.45
1:R:37:TYR:CD2	1:R:85:PHE:HB2	2.52	0.45
1:I:9:LYS:HB3	1:I:100:LEU:HD11	1.99	0.45
1:K:87:ASN:HB3	1:Q:87:ASN:CB	2.47	0.45
1:D:14:TYR:HB2	1:D:97:LEU:HB3	1.98	0.44
1:M:9:LYS:HB3	1:M:100:LEU:HD11	1.98	0.44
1:F:16[B]:ASP:OD2	1:F:68:LYS:HD2	2.16	0.44
1:C:58:HIS:HB3	1:C:68:LYS:O	2.17	0.44
1:O:12:LYS:NZ	4:O:203:SO4:O2	2.31	0.44
1:E:76:ILE:HG23	1:E:103:ILE:HD11	1.99	0.44
1:K:7:ASN:HA	1:K:104:GLU:HA	2.00	0.44
1:L:56:GLU:H	1:L:56:GLU:HG3	1.59	0.44
1:F:17:ASN:O	1:B:65:MET:HE1	2.18	0.44
1:M:48:ALA:HB2	1:O:46:LYS:HG2	1.99	0.44
1:E:12:LYS:HB2	1:E:99:THR:OG1	2.17	0.44
1:G:14:TYR:HB2	1:G:97:LEU:HB3	2.00	0.44
1:B:12:LYS:HB2	1:B:99:THR:OG1	2.18	0.44
1:K:77:ASP:HB3	1:K:82:ILE:HG12	1.99	0.44
1:M:52:GLY:O	1:M:55:SER:OG	2.36	0.44
1:G:14:TYR:CD2	1:G:72:ILE:HD12	2.52	0.43
1:F:4:TYR:HE1	1:F:104:GLU:OE2	2.01	0.43
1:Q:97:LEU:HD22	2:Q:201:CMP:C5	2.53	0.43
1:K:31:LEU:HD22	1:L:51:MET:HE3	2.00	0.43
1:R:65:MET:O	1:R:65:MET:HE3	2.18	0.43
1:E:43:THR:OG1	2:F:201[B]:CMP:N7	2.51	0.43
1:G:44:VAL:HG22	1:G:73:ILE:HG13	2.00	0.43
1:Q:76:ILE:N	2:R:202[B]:CMP:HN62	2.15	0.43
2:D:201[A]:CMP:H8	1:F:43:THR:OG1	2.19	0.43
1:E:13:ILE:HG22	1:E:15:ILE:HG23	2.00	0.43
1:P:76:ILE:HG23	1:P:103:ILE:HD11	2.01	0.43
1:R:14:TYR:HB3	2:R:202[B]:CMP:H2'	2.00	0.43
1:F:105:VAL:HG12	1:F:106:LEU:N	2.34	0.43
1:M:51:MET:HG3	1:O:42:ALA:H	1.83	0.43
1:E:28:GLN:HG2	1:E:32:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:VAL:HA	1:E:72:ILE:O	2.19	0.43
1:E:46:LYS:HE3	1:E:46:LYS:HB2	1.72	0.43
1:K:54:HIS:O	1:K:55:SER:C	2.61	0.43
1:G:51:MET:HE3	1:G:57:ILE:HG13	2.01	0.42
1:G:74:GLU:O	2:G:201:CMP:H2	2.19	0.42
1:I:18:ASP:HB3	1:I:68:LYS:HD2	2.01	0.42
1:H:54:HIS:O	1:H:56:GLU:N	2.46	0.42
1:K:10:LYS:HE2	1:K:103:ILE:HG21	2.00	0.42
1:E:63:TRP:HH2	1:A:57:ILE:HG21	1.84	0.42
1:B:10:LYS:HB3	1:B:101:GLU:HG2	2.02	0.42
1:G:11:LEU:O	1:G:74:GLU:HA	2.19	0.42
1:E:54:HIS:O	1:E:56:GLU:N	2.52	0.42
1:F:94:THR:OG1	1:F:95:GLU:N	2.52	0.42
1:G:58:HIS:HB3	1:G:68:LYS:O	2.19	0.42
1:H:4:TYR:O	1:H:106:LEU:HD12	2.20	0.42
1:H:89:ILE:HB	1:H:92:MET:HE2	2.00	0.42
1:N:44:VAL:HG22	1:N:73:ILE:HG12	2.02	0.42
1:H:55:SER:O	1:H:56:GLU:HB3	2.19	0.42
1:D:14:TYR:HB3	2:D:201[A]:CMP:O2'	2.20	0.42
1:F:65:MET:HE1	1:B:17:ASN:O	2.19	0.42
1:I:77:ASP:HB3	1:I:82:ILE:HG12	2.02	0.42
1:M:60:PHE:HE2	1:M:62:VAL:HG22	1.83	0.42
1:N:13:ILE:HG22	1:N:15:ILE:HG23	2.01	0.42
1:R:59:THR:OG1	1:R:60:PHE:N	2.53	0.42
1:G:31:LEU:HB3	1:H:51:MET:HE3	2.01	0.42
1:N:47:ALA:HB3	1:N:70:PRO:HB2	2.01	0.42
1:A:24:LYS:HG3	1:A:25:PRO:HD2	2.02	0.42
1:M:57:ILE:HG22	1:M:59:THR:HG23	2.02	0.42
1:J:57:ILE:HG22	1:J:59:THR:HG23	2.01	0.41
1:R:24:LYS:HD3	1:R:28:GLN:HG2	2.02	0.41
1:B:18:ASP:OD2	1:B:68:LYS:HG2	2.20	0.41
1:N:44:VAL:HA	1:N:72:ILE:O	2.21	0.41
1:E:51:MET:HE2	1:E:51:MET:HB3	1.96	0.41
1:K:76:ILE:CG2	1:K:103:ILE:HD11	2.51	0.41
1:D:101:GLU:HB3	1:F:103:ILE:HG22	2.02	0.41
1:C:77:ASP:HB3	1:C:82:ILE:HG12	2.02	0.41
1:G:61:ASN:HB3	1:G:64:SER:OG	2.20	0.41
1:E:41:GLY:HA3	1:F:52:GLY:HA2	2.02	0.41
1:F:70:PRO:HG3	2:F:201[B]:CMP:O1P	2.20	0.41
1:K:77:ASP:OD1	1:K:78:SER:N	2.53	0.41
1:N:81:LYS:HE3	1:N:81:LYS:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:LYS:HD2	1:G:24:LYS:HA	1.80	0.41
1:H:9:LYS:HB3	1:H:100:LEU:HD11	2.03	0.41
1:H:94:THR:OG1	1:H:95:GLU:N	2.52	0.41
1:J:12:LYS:HB2	1:J:99:THR:OG1	2.21	0.41
1:L:37:TYR:CD2	1:L:85:PHE:HB2	2.56	0.41
1:N:5:LEU:O	1:N:8:ARG:NH2	2.41	0.41
1:N:12:LYS:HB2	1:N:99:THR:OG1	2.21	0.41
1:P:9:LYS:HB3	1:P:100:LEU:HD11	2.02	0.41
1:B:51:MET:HG2	1:B:57:ILE:HG12	2.03	0.41
1:P:60:PHE:HE2	1:P:62:VAL:HG22	1.84	0.41
1:I:57:ILE:HG22	1:I:59:THR:HG23	2.02	0.40
1:K:76:ILE:HD13	1:L:99:THR:HG21	2.02	0.40
1:B:86:LEU:HD21	1:B:98:VAL:HG11	2.02	0.40
1:N:41:GLY:HA3	2:O:202[B]:CMP:C2	2.57	0.40
2:D:201[A]:CMP:HN62	1:F:76:ILE:N	2.05	0.40
1:A:34:ALA:HB2	1:A:85:PHE:CZ	2.56	0.40
1:B:58:HIS:HB3	1:B:68:LYS:O	2.22	0.40
1:R:12:LYS:NZ	4:R:203:SO4:O4	2.49	0.40
1:P:24:LYS:HG3	1:P:25:PRO:HD2	2.04	0.40
1:D:35:LYS:HA	1:D:35:LYS:HD2	1.93	0.40
1:A:76:ILE:HG23	1:A:103:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	103/122 (84%)	92 (89%)	10 (10%)	1 (1%)	12 5
1	B	106/122 (87%)	94 (89%)	10 (9%)	2 (2%)	6 1
1	C	98/122 (80%)	94 (96%)	3 (3%)	1 (1%)	12 5
1	D	100/122 (82%)	96 (96%)	3 (3%)	1 (1%)	12 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	101/122 (83%)	92 (91%)	7 (7%)	2 (2%)	6 1
1	F	108/122 (88%)	99 (92%)	7 (6%)	2 (2%)	6 1
1	G	101/122 (83%)	89 (88%)	11 (11%)	1 (1%)	12 5
1	H	105/122 (86%)	96 (91%)	9 (9%)	0	100 100
1	I	98/122 (80%)	93 (95%)	4 (4%)	1 (1%)	12 5
1	J	99/122 (81%)	92 (93%)	5 (5%)	2 (2%)	6 1
1	K	99/122 (81%)	90 (91%)	7 (7%)	2 (2%)	6 1
1	L	108/122 (88%)	99 (92%)	7 (6%)	2 (2%)	6 1
1	M	99/122 (81%)	91 (92%)	5 (5%)	3 (3%)	3 0
1	N	99/122 (81%)	88 (89%)	8 (8%)	3 (3%)	3 0
1	O	104/122 (85%)	100 (96%)	4 (4%)	0	100 100
1	P	100/122 (82%)	94 (94%)	5 (5%)	1 (1%)	12 5
1	Q	100/122 (82%)	90 (90%)	8 (8%)	2 (2%)	6 1
1	R	107/122 (88%)	99 (92%)	7 (6%)	1 (1%)	14 6
All	All	1835/2196 (84%)	1688 (92%)	120 (6%)	27 (2%)	8 2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	55	SER
1	A	53	ALA
1	K	53	ALA
1	K	55	SER
1	Q	53	ALA
1	Q	55	SER
1	G	53	ALA
1	N	54	HIS
1	N	56	GLU
1	R	54	HIS
1	D	22	ASN
1	E	22	ASN
1	B	53	ALA
1	B	55	SER
1	L	4	TYR
1	L	94	THR
1	M	53	ALA
1	N	55	SER

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Mol	Chain	Res	Type
1	P	53	ALA
1	F	56	GLU
1	C	22	ASN
1	I	22	ASN
1	J	22	ASN
1	M	65	MET
1	F	54	HIS
1	J	53	ALA
1	M	52	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/103 (85%)	74 (84%)	14 (16%)	2 0
1	B	89/103 (86%)	83 (93%)	6 (7%)	15 4
1	C	82/103 (80%)	80 (98%)	2 (2%)	43 31
1	D	85/103 (82%)	82 (96%)	3 (4%)	32 18
1	E	86/103 (84%)	82 (95%)	4 (5%)	23 10
1	F	92/103 (89%)	81 (88%)	11 (12%)	5 0
1	G	86/103 (84%)	83 (96%)	3 (4%)	32 18
1	H	90/103 (87%)	81 (90%)	9 (10%)	7 1
1	I	82/103 (80%)	80 (98%)	2 (2%)	43 31
1	J	83/103 (81%)	77 (93%)	6 (7%)	13 3
1	K	84/103 (82%)	81 (96%)	3 (4%)	31 17
1	L	91/103 (88%)	84 (92%)	7 (8%)	12 3
1	M	82/103 (80%)	77 (94%)	5 (6%)	17 5
1	N	82/103 (80%)	78 (95%)	4 (5%)	22 9
1	O	88/103 (85%)	75 (85%)	13 (15%)	3 0
1	P	85/103 (82%)	80 (94%)	5 (6%)	18 6
1	Q	82/103 (80%)	79 (96%)	3 (4%)	30 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	91/103 (88%)	85 (93%)	6 (7%)	15 4
All	All	1548/1854 (84%)	1442 (93%)	106 (7%)	15 4

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	MET
1	D	68	LYS
1	D	103	ILE
1	E	8	ARG
1	E	11	LEU
1	E	46	LYS
1	E	64	SER
1	F	16[A]	ASP
1	F	16[B]	ASP
1	F	24	LYS
1	F	35	LYS
1	F	51	MET
1	F	54	HIS
1	F	56	GLU
1	F	62	VAL
1	F	69	LEU
1	F	95	GLU
1	F	106	LEU
1	C	94	THR
1	C	95	GLU
1	A	5	LEU
1	A	8	ARG
1	A	20	ARG
1	A	24	LYS
1	A	31	LEU
1	A	32	HIS
1	A	35	LYS
1	A	46	LYS
1	A	51	MET
1	A	57	ILE
1	A	65	MET
1	A	90	ASP
1	A	105	VAL
1	A	107	LEU
1	B	5	LEU
1	B	21	SER

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Mol	Chain	Res	Type
1	B	56	GLU
1	B	68	LYS
1	B	101	GLU
1	B	106	LEU
1	I	51	MET
1	I	55	SER
1	G	35	LYS
1	G	56	GLU
1	G	107	LEU
1	H	5	LEU
1	H	15	ILE
1	H	16	ASP
1	H	22	ASN
1	H	51	MET
1	H	56	GLU
1	H	103	ILE
1	H	104	GLU
1	H	107	LEU
1	J	18[A]	ASP
1	J	18[B]	ASP
1	J	21	SER
1	J	62	VAL
1	J	92	MET
1	J	103	ILE
1	K	56	GLU
1	K	57	ILE
1	K	100	LEU
1	L	5	LEU
1	L	46	LYS
1	L	55	SER
1	L	56	GLU
1	L	62	VAL
1	L	95	GLU
1	L	101	GLU
1	M	20	ARG
1	M	35	LYS
1	M	92	MET
1	M	102	ASP
1	M	103	ILE
1	N	31	LEU
1	N	46	LYS
1	N	57	ILE

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Mol	Chain	Res	Type
1	N	77	ASP
1	O	5	LEU
1	O	16	ASP
1	O	18	ASP
1	O	22	ASN
1	O	46	LYS
1	O	51	MET
1	O	55	SER
1	O	56	GLU
1	O	83	ARG
1	O	101	GLU
1	O	103	ILE
1	O	107	LEU
1	O	109	LYS
1	P	24	LYS
1	P	51	MET
1	P	55	SER
1	P	59	THR
1	P	65	MET
1	Q	57	ILE
1	Q	66	SER
1	Q	68	LYS
1	R	16	ASP
1	R	18[A]	ASP
1	R	18[B]	ASP
1	R	54	HIS
1	R	99	THR
1	R	102	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	22	ASN
1	B	58	HIS
1	G	32	HIS
1	L	22	ASN
1	P	33	GLN
1	R	22	ASN
1	R	32	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 6 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CMP	L	201	-	25,25,25	1.71	7 (28%)	37,39,39	1.99	10 (27%)
4	SO4	F	202	3	4,4,4	0.67	0	6,6,6	0.08	0
4	SO4	J	202	3	4,4,4	0.66	0	6,6,6	0.07	0
2	CMP	A	201	-	25,25,25	1.75	7 (28%)	37,39,39	2.13	13 (35%)
2	CMP	L	202[B]	-	25,25,25	1.80	6 (24%)	37,39,39	2.41	14 (37%)
2	CMP	M	201	-	25,25,25	1.77	8 (32%)	37,39,39	2.14	13 (35%)
2	CMP	H	201	-	25,25,25	1.71	8 (32%)	37,39,39	1.96	10 (27%)
4	SO4	R	203	3	4,4,4	0.67	0	6,6,6	0.07	0
2	CMP	B	201	-	25,25,25	1.74	7 (28%)	37,39,39	1.96	9 (24%)
2	CMP	O	202[A]	-	25,25,25	1.74	7 (28%)	37,39,39	1.92	9 (24%)
2	CMP	D	201[A]	-	25,25,25	1.77	8 (32%)	37,39,39	2.06	9 (24%)
4	SO4	G	203	3	4,4,4	0.66	0	6,6,6	0.09	0
2	CMP	F	201[A]	-	25,25,25	1.77	9 (36%)	37,39,39	2.11	12 (32%)
2	CMP	B	202	-	25,25,25	1.79	7 (28%)	37,39,39	2.07	11 (29%)
2	CMP	R	201	-	25,25,25	1.69	6 (24%)	37,39,39	1.97	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CMP	G	201	-	25,25,25	1.77	8 (32%)	37,39,39	1.93	9 (24%)
2	CMP	R	202[A]	-	25,25,25	1.76	7 (28%)	37,39,39	1.96	10 (27%)
2	CMP	O	202[B]	-	25,25,25	1.90	8 (32%)	37,39,39	2.40	13 (35%)
2	CMP	D	201[B]	-	25,25,25	1.74	8 (32%)	37,39,39	1.99	9 (24%)
2	CMP	O	201	-	25,25,25	1.72	8 (32%)	37,39,39	1.96	9 (24%)
2	CMP	L	202[A]	-	25,25,25	1.77	9 (36%)	37,39,39	2.07	11 (29%)
2	CMP	E	201	-	25,25,25	1.76	8 (32%)	37,39,39	1.99	10 (27%)
2	CMP	I	201	-	25,25,25	1.77	8 (32%)	37,39,39	2.14	11 (29%)
2	CMP	Q	201	-	25,25,25	1.72	7 (28%)	37,39,39	2.10	13 (35%)
2	CMP	F	201[B]	-	25,25,25	1.76	7 (28%)	37,39,39	2.17	12 (32%)
4	SO4	O	203	3	4,4,4	0.66	0	6,6,6	0.06	0
4	SO4	B	204	3	4,4,4	0.66	0	6,6,6	0.08	0
2	CMP	J	201	-	25,25,25	1.77	8 (32%)	37,39,39	1.99	10 (27%)
2	CMP	R	202[B]	-	25,25,25	1.75	8 (32%)	37,39,39	2.02	11 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	L	201	-	-	0/4/31/31	0/4/4/4
2	CMP	A	201	-	-	0/4/31/31	0/4/4/4
2	CMP	L	202[B]	-	-	0/4/31/31	0/4/4/4
2	CMP	M	201	-	-	0/4/31/31	0/4/4/4
2	CMP	H	201	-	-	0/4/31/31	0/4/4/4
2	CMP	B	201	-	-	0/4/31/31	0/4/4/4
2	CMP	O	202[A]	-	-	0/4/31/31	0/4/4/4
2	CMP	D	201[A]	-	-	2/4/31/31	0/4/4/4
2	CMP	F	201[A]	-	-	0/4/31/31	0/4/4/4
2	CMP	B	202	-	-	2/4/31/31	0/4/4/4
2	CMP	R	201	-	-	0/4/31/31	0/4/4/4
2	CMP	G	201	-	-	0/4/31/31	0/4/4/4
2	CMP	R	202[A]	-	-	0/4/31/31	0/4/4/4
2	CMP	O	202[B]	-	-	0/4/31/31	0/4/4/4
2	CMP	D	201[B]	-	-	0/4/31/31	0/4/4/4
2	CMP	O	201	-	-	0/4/31/31	0/4/4/4
2	CMP	L	202[A]	-	-	0/4/31/31	0/4/4/4
2	CMP	E	201	-	-	0/4/31/31	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	I	201	-	-	0/4/31/31	0/4/4/4
2	CMP	Q	201	-	-	0/4/31/31	0/4/4/4
2	CMP	F	201[B]	-	-	2/4/31/31	0/4/4/4
2	CMP	J	201	-	-	0/4/31/31	0/4/4/4
2	CMP	R	202[B]	-	-	2/4/31/31	0/4/4/4

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	CMP	C5-C4	5.12	1.48	1.39
2	F	201[B]	CMP	C5-C4	4.96	1.47	1.39
2	B	201	CMP	C5-C4	4.88	1.47	1.39
2	J	201	CMP	C5-C4	4.79	1.47	1.39
2	D	201[A]	CMP	C5-C4	4.77	1.47	1.39
2	G	201	CMP	C5-C4	4.75	1.47	1.39
2	E	201	CMP	C5-C4	4.74	1.47	1.39
2	O	201	CMP	C5-C4	4.73	1.47	1.39
2	R	202[A]	CMP	C5-C4	4.68	1.47	1.39
2	H	201	CMP	C5-C4	4.67	1.47	1.39
2	I	201	CMP	C5-C4	4.66	1.47	1.39
2	A	201	CMP	C5-C4	4.65	1.47	1.39
2	M	201	CMP	C5-C4	4.65	1.47	1.39
2	L	202[A]	CMP	C5-C4	4.64	1.47	1.39
2	Q	201	CMP	C5-C4	4.64	1.47	1.39
2	D	201[B]	CMP	C5-C4	4.64	1.47	1.39
2	O	202[A]	CMP	C5-C4	4.63	1.47	1.39
2	F	201[A]	CMP	C5-C4	4.60	1.47	1.39
2	L	201	CMP	C5-C4	4.57	1.47	1.39
2	R	201	CMP	C5-C4	4.56	1.47	1.39
2	L	202[B]	CMP	C5-C4	4.46	1.47	1.39
2	R	202[B]	CMP	C5-C4	4.38	1.46	1.39
2	O	202[B]	CMP	C5-C4	4.35	1.46	1.39
2	O	202[B]	CMP	P-O5'	4.01	1.62	1.57
2	O	202[B]	CMP	P-O3'	3.94	1.64	1.57
2	L	202[B]	CMP	P-O5'	3.51	1.61	1.57
2	L	202[B]	CMP	P-O3'	3.35	1.63	1.57
2	B	201	CMP	P-O5'	3.29	1.61	1.57
2	F	201[A]	CMP	P-O5'	3.25	1.61	1.57
2	L	202[A]	CMP	P-O5'	3.24	1.61	1.57
2	R	202[B]	CMP	P-O3'	3.23	1.63	1.57
2	A	201	CMP	P-O5'	3.18	1.61	1.57
2	M	201	CMP	P-O5'	3.14	1.61	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	CMP	P-O5'	3.13	1.61	1.57
2	G	201	CMP	P-O5'	3.10	1.61	1.57
2	I	201	CMP	P-O5'	3.10	1.61	1.57
2	R	202[A]	CMP	P-O3'	3.10	1.62	1.57
2	R	201	CMP	P-O5'	3.08	1.61	1.57
2	O	201	CMP	P-O5'	3.07	1.61	1.57
2	R	202[A]	CMP	P-O5'	3.06	1.61	1.57
2	J	201	CMP	P-O3'	3.06	1.62	1.57
2	F	201[B]	CMP	P-O5'	3.05	1.61	1.57
2	D	201[B]	CMP	P-O5'	3.05	1.61	1.57
2	H	201	CMP	P-O5'	3.05	1.61	1.57
2	F	201[A]	CMP	P-O3'	3.03	1.62	1.57
2	D	201[A]	CMP	P-O5'	3.02	1.61	1.57
2	Q	201	CMP	P-O5'	3.02	1.61	1.57
2	B	202	CMP	P-O3'	3.00	1.62	1.57
2	O	202[A]	CMP	P-O5'	2.99	1.61	1.57
2	G	201	CMP	P-O3'	2.98	1.62	1.57
2	B	202	CMP	P-O5'	2.97	1.61	1.57
2	E	201	CMP	P-O3'	2.96	1.62	1.57
2	L	202[A]	CMP	P-O3'	2.94	1.62	1.57
2	I	201	CMP	P-O3'	2.90	1.62	1.57
2	D	201[A]	CMP	P-O3'	2.90	1.62	1.57
2	M	201	CMP	C5-C6	2.89	1.49	1.41
2	E	201	CMP	P-O5'	2.88	1.61	1.57
2	O	202[A]	CMP	P-O3'	2.85	1.62	1.57
2	D	201[B]	CMP	C5-C6	2.84	1.48	1.41
2	A	201	CMP	C5-C6	2.83	1.48	1.41
2	F	201[B]	CMP	C5-C6	2.80	1.48	1.41
2	O	202[A]	CMP	C5-C6	2.79	1.48	1.41
2	L	201	CMP	C5-C6	2.79	1.48	1.41
2	R	202[B]	CMP	P-O5'	2.79	1.60	1.57
2	G	201	CMP	C5-C6	2.78	1.48	1.41
2	J	201	CMP	P-O5'	2.78	1.60	1.57
2	F	201[A]	CMP	C5-C6	2.78	1.48	1.41
2	E	201	CMP	C5-C6	2.78	1.48	1.41
2	D	201[B]	CMP	P-O3'	2.76	1.62	1.57
2	R	202[A]	CMP	C5-C6	2.76	1.48	1.41
2	Q	201	CMP	C5-C6	2.75	1.48	1.41
2	J	201	CMP	C5-C6	2.75	1.48	1.41
2	L	202[A]	CMP	C5-C6	2.74	1.48	1.41
2	R	201	CMP	C5-C6	2.73	1.48	1.41
2	H	201	CMP	C5-C6	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	201	CMP	P-O3'	2.71	1.62	1.57
2	L	202[B]	CMP	C5-C6	2.70	1.48	1.41
2	R	202[B]	CMP	C5-C6	2.70	1.48	1.41
2	O	201	CMP	C5-C6	2.70	1.48	1.41
2	I	201	CMP	C5-C6	2.69	1.48	1.41
2	O	202[B]	CMP	C5-C6	2.68	1.48	1.41
2	A	201	CMP	P-O3'	2.67	1.62	1.57
2	B	201	CMP	C5-C6	2.64	1.48	1.41
2	B	202	CMP	C5-C6	2.62	1.48	1.41
2	F	201[B]	CMP	P-O3'	2.58	1.62	1.57
2	O	201	CMP	P-O3'	2.55	1.62	1.57
2	B	201	CMP	P-O3'	2.54	1.62	1.57
2	Q	201	CMP	P-O3'	2.53	1.62	1.57
2	M	201	CMP	O3'-C3'	-2.52	1.40	1.44
2	B	202	CMP	C5-N7	-2.50	1.34	1.39
2	I	201	CMP	O3'-C3'	-2.49	1.40	1.44
2	Q	201	CMP	O3'-C3'	-2.49	1.40	1.44
2	A	201	CMP	O3'-C3'	-2.48	1.40	1.44
2	D	201[A]	CMP	C5-C6	2.48	1.47	1.41
2	J	201	CMP	C8-N7	2.46	1.36	1.31
2	H	201	CMP	P-O3'	2.46	1.61	1.57
2	L	202[A]	CMP	C8-N7	2.45	1.36	1.31
2	D	201[A]	CMP	O5'-C5'	-2.45	1.42	1.46
2	D	201[A]	CMP	C5-N7	-2.45	1.34	1.39
2	M	201	CMP	C8-N7	2.45	1.36	1.31
2	O	202[A]	CMP	C8-N7	2.44	1.36	1.31
2	A	201	CMP	C8-N7	2.44	1.36	1.31
2	G	201	CMP	C8-N7	2.44	1.36	1.31
2	F	201[A]	CMP	C8-N7	2.44	1.36	1.31
2	R	202[A]	CMP	C8-N7	2.43	1.36	1.31
2	L	201	CMP	P-O3'	2.42	1.61	1.57
2	I	201	CMP	C8-N7	2.42	1.36	1.31
2	L	202[B]	CMP	C8-N7	2.42	1.36	1.31
2	F	201[B]	CMP	C5-N7	-2.41	1.34	1.39
2	D	201[B]	CMP	C8-N7	2.41	1.36	1.31
2	O	202[B]	CMP	C8-N7	2.40	1.36	1.31
2	R	202[B]	CMP	C8-N7	2.40	1.36	1.31
2	O	201	CMP	C8-N7	2.40	1.36	1.31
2	H	201	CMP	C8-N7	2.39	1.36	1.31
2	G	201	CMP	C5-N7	-2.39	1.34	1.39
2	E	201	CMP	C8-N7	2.39	1.36	1.31
2	R	201	CMP	P-O3'	2.38	1.61	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	201	CMP	C8-N7	2.38	1.36	1.31
2	B	201	CMP	O3'-C3'	-2.38	1.41	1.44
2	R	202[B]	CMP	O5'-C5'	-2.37	1.42	1.46
2	B	201	CMP	C8-N7	2.36	1.36	1.31
2	Q	201	CMP	C8-N7	2.34	1.36	1.31
2	L	201	CMP	C8-N7	2.34	1.36	1.31
2	R	202[B]	CMP	C4-N9	-2.33	1.32	1.37
2	L	201	CMP	O3'-C3'	-2.31	1.41	1.44
2	H	201	CMP	O3'-C3'	-2.30	1.41	1.44
2	O	202[B]	CMP	C8-N9	-2.30	1.33	1.37
2	J	201	CMP	O5'-C5'	-2.28	1.42	1.46
2	F	201[B]	CMP	C8-N7	2.27	1.36	1.31
2	F	201[B]	CMP	O3'-C3'	-2.27	1.41	1.44
2	R	201	CMP	O3'-C3'	-2.26	1.41	1.44
2	O	201	CMP	O3'-C3'	-2.25	1.41	1.44
2	D	201[B]	CMP	C5-N7	-2.21	1.35	1.39
2	E	201	CMP	O3'-C3'	-2.21	1.41	1.44
2	I	201	CMP	O5'-C5'	-2.21	1.43	1.46
2	E	201	CMP	O5'-C5'	-2.20	1.43	1.46
2	E	201	CMP	C5-N7	-2.20	1.35	1.39
2	J	201	CMP	C5-N7	-2.19	1.35	1.39
2	L	202[A]	CMP	O5'-C5'	-2.19	1.43	1.46
2	J	201	CMP	O3'-C3'	-2.18	1.41	1.44
2	L	202[A]	CMP	C5-N7	-2.18	1.35	1.39
2	O	202[A]	CMP	C5-N7	-2.18	1.35	1.39
2	L	202[B]	CMP	C5-N7	-2.17	1.35	1.39
2	F	201[A]	CMP	O3'-C3'	-2.15	1.41	1.44
2	B	202	CMP	O5'-C5'	-2.14	1.43	1.46
2	F	201[A]	CMP	C5-N7	-2.14	1.35	1.39
2	R	202[A]	CMP	O5'-C5'	-2.14	1.43	1.46
2	L	202[A]	CMP	O3'-C3'	-2.14	1.41	1.44
2	L	201	CMP	C5-N7	-2.14	1.35	1.39
2	R	202[A]	CMP	C5-N7	-2.13	1.35	1.39
2	D	201[B]	CMP	O3'-C3'	-2.12	1.41	1.44
2	A	201	CMP	C5-N7	-2.11	1.35	1.39
2	F	201[A]	CMP	O5'-C5'	-2.11	1.43	1.46
2	D	201[A]	CMP	C8-N7	2.10	1.35	1.31
2	O	202[B]	CMP	C4-N9	-2.10	1.33	1.37
2	O	202[B]	CMP	C5-N7	-2.09	1.35	1.39
2	M	201	CMP	O5'-C5'	-2.09	1.43	1.46
2	O	202[A]	CMP	O5'-C5'	-2.08	1.43	1.46
2	R	202[B]	CMP	C5-N7	-2.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	201	CMP	C5-N7	-2.08	1.35	1.39
2	B	201	CMP	C5-N7	-2.07	1.35	1.39
2	F	201[A]	CMP	C4-N9	-2.06	1.33	1.37
2	G	201	CMP	O5'-C5'	-2.05	1.43	1.46
2	O	201	CMP	O5'-C5'	-2.05	1.43	1.46
2	B	202	CMP	O3'-C3'	-2.04	1.41	1.44
2	D	201[A]	CMP	C8-N9	-2.03	1.34	1.37
2	O	201	CMP	C5-N7	-2.03	1.35	1.39
2	Q	201	CMP	C5-N7	-2.03	1.35	1.39
2	L	202[A]	CMP	C4-N9	-2.03	1.33	1.37
2	H	201	CMP	O5'-C5'	-2.03	1.43	1.46
2	D	201[B]	CMP	O5'-C5'	-2.02	1.43	1.46
2	H	201	CMP	C5-N7	-2.02	1.35	1.39
2	M	201	CMP	C5-N7	-2.02	1.35	1.39
2	G	201	CMP	C4-N9	-2.01	1.33	1.37

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	202[B]	CMP	O3'-C3'-C4'	-7.35	105.17	110.71
2	F	201[B]	CMP	C5-C4-N3	-6.54	117.71	126.72
2	B	202	CMP	C5-C4-N3	-6.54	117.71	126.72
2	D	201[A]	CMP	C5-C4-N3	-6.23	118.14	126.72
2	L	202[B]	CMP	O3'-C3'-C4'	-5.94	106.23	110.71
2	D	201[B]	CMP	C5-C4-N3	-5.92	118.57	126.72
2	G	201	CMP	C5-C4-N3	-5.88	118.62	126.72
2	B	201	CMP	C5-C4-N3	-5.86	118.64	126.72
2	I	201	CMP	C5-C4-N3	-5.86	118.64	126.72
2	E	201	CMP	C5-C4-N3	-5.84	118.67	126.72
2	O	201	CMP	C5-C4-N3	-5.83	118.68	126.72
2	J	201	CMP	C5-C4-N3	-5.79	118.75	126.72
2	R	202[A]	CMP	C5-C4-N3	-5.77	118.77	126.72
2	O	202[A]	CMP	C5-C4-N3	-5.77	118.78	126.72
2	R	201	CMP	C5-C4-N3	-5.76	118.78	126.72
2	L	201	CMP	C5-C4-N3	-5.75	118.79	126.72
2	Q	201	CMP	C5-C4-N3	-5.69	118.88	126.72
2	F	201[A]	CMP	C5-C4-N3	-5.66	118.92	126.72
2	L	202[A]	CMP	C5-C4-N3	-5.64	118.95	126.72
2	A	201	CMP	C5-C4-N3	-5.61	119.00	126.72
2	H	201	CMP	C5-C4-N3	-5.49	119.15	126.72
2	L	202[B]	CMP	C5-C4-N3	-5.49	119.15	126.72
2	M	201	CMP	C5-C4-N3	-5.45	119.22	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	202[B]	CMP	C5-C4-N3	-5.38	119.31	126.72
2	D	201[A]	CMP	N3-C4-N9	5.28	136.15	127.17
2	B	202	CMP	N3-C4-N9	5.24	136.08	127.17
2	R	202[B]	CMP	C5-C4-N3	-5.12	119.67	126.72
2	F	201[B]	CMP	N3-C4-N9	5.10	135.84	127.17
2	L	202[B]	CMP	O5'-P-O3'	5.05	112.47	105.70
2	F	201[A]	CMP	O5'-P-O3'	4.82	112.16	105.70
2	I	201	CMP	O5'-P-O3'	4.80	112.12	105.70
2	E	201	CMP	N3-C4-N9	4.61	135.01	127.17
2	I	201	CMP	N3-C4-N9	4.55	134.91	127.17
2	B	201	CMP	N3-C4-N9	4.53	134.88	127.17
2	M	201	CMP	O5'-P-O3'	4.51	111.74	105.70
2	L	201	CMP	N3-C4-N9	4.49	134.80	127.17
2	O	201	CMP	N3-C4-N9	4.48	134.79	127.17
2	Q	201	CMP	N3-C4-N9	4.42	134.68	127.17
2	R	201	CMP	N3-C4-N9	4.41	134.67	127.17
2	J	201	CMP	N3-C4-N9	4.38	134.62	127.17
2	O	202[B]	CMP	N3-C4-N9	4.37	134.60	127.17
2	D	201[B]	CMP	N3-C4-N9	4.37	134.59	127.17
2	L	202[B]	CMP	N3-C4-N9	4.33	134.53	127.17
2	A	201	CMP	O5'-P-O3'	4.30	111.45	105.70
2	A	201	CMP	N3-C4-N9	4.28	134.44	127.17
2	R	202[A]	CMP	N3-C4-N9	4.28	134.44	127.17
2	H	201	CMP	N3-C4-N9	4.26	134.41	127.17
2	O	202[A]	CMP	N3-C4-N9	4.23	134.36	127.17
2	F	201[A]	CMP	N3-C4-N9	4.21	134.32	127.17
2	L	202[A]	CMP	N3-C4-N9	4.19	134.30	127.17
2	G	201	CMP	N3-C4-N9	4.17	134.25	127.17
2	M	201	CMP	N3-C4-N9	4.09	134.12	127.17
2	L	202[A]	CMP	O5'-P-O3'	4.08	111.16	105.70
2	M	201	CMP	C4-C5-N7	-4.01	105.99	110.58
2	R	202[B]	CMP	N3-C4-N9	4.00	133.98	127.17
2	R	202[B]	CMP	O2P-P-O1P	3.89	120.51	108.56
2	G	201	CMP	C4-C5-N7	-3.87	106.16	110.58
2	Q	201	CMP	C4-C5-N7	-3.84	106.19	110.58
2	R	202[A]	CMP	C4-C5-N7	-3.82	106.22	110.58
2	D	201[B]	CMP	C4-C5-N7	-3.81	106.22	110.58
2	O	201	CMP	C2-N3-C4	3.81	121.13	111.83
2	F	201[B]	CMP	C2-N3-C4	3.80	121.11	111.83
2	A	201	CMP	C4-C5-N7	-3.79	106.24	110.58
2	O	202[A]	CMP	C4-C5-N7	-3.78	106.26	110.58
2	F	201[A]	CMP	C4-C5-N7	-3.78	106.26	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	201	CMP	C4-C5-N7	-3.77	106.27	110.58
2	R	201	CMP	C2-N3-C4	3.75	120.99	111.83
2	D	201[A]	CMP	C2-N3-C4	3.75	120.98	111.83
2	L	202[A]	CMP	C4-C5-N7	-3.75	106.30	110.58
2	I	201	CMP	C2-N3-C4	3.74	120.97	111.83
2	D	201[B]	CMP	C2-N3-C4	3.74	120.97	111.83
2	A	201	CMP	C2-N3-C4	3.72	120.91	111.83
2	B	201	CMP	C2-N3-C4	3.72	120.91	111.83
2	B	202	CMP	C2-N3-C4	3.71	120.89	111.83
2	L	201	CMP	C2-N3-C4	3.71	120.88	111.83
2	R	202[A]	CMP	C2-N3-C4	3.70	120.88	111.83
2	E	201	CMP	C2-N3-C4	3.68	120.81	111.83
2	Q	201	CMP	C2-N3-C4	3.67	120.79	111.83
2	L	202[A]	CMP	C2-N3-C4	3.67	120.79	111.83
2	O	202[B]	CMP	C2-N3-C4	3.67	120.78	111.83
2	H	201	CMP	C2-N3-C4	3.66	120.77	111.83
2	J	201	CMP	C2-N3-C4	3.65	120.75	111.83
2	I	201	CMP	C4-C5-N7	-3.65	106.41	110.58
2	L	202[B]	CMP	O2P-P-O1P	3.65	119.78	108.56
2	O	202[A]	CMP	C2-N3-C4	3.65	120.73	111.83
2	L	202[B]	CMP	C2-N3-C4	3.64	120.73	111.83
2	L	201	CMP	C4-C5-N7	-3.64	106.42	110.58
2	F	201[A]	CMP	C2-N3-C4	3.64	120.71	111.83
2	G	201	CMP	C2-N3-C4	3.62	120.67	111.83
2	M	201	CMP	C2-N3-C4	3.62	120.67	111.83
2	E	201	CMP	C4-C5-N7	-3.62	106.45	110.58
2	R	201	CMP	C4-C5-N7	-3.59	106.48	110.58
2	L	202[A]	CMP	O2P-P-O1P	3.59	119.58	108.56
2	R	202[B]	CMP	C2-N3-C4	3.59	120.59	111.83
2	R	202[B]	CMP	C4-C5-N7	-3.56	106.51	110.58
2	D	201[A]	CMP	O2P-P-O1P	3.56	119.50	108.56
2	B	201	CMP	C4-C5-N7	-3.55	106.52	110.58
2	H	201	CMP	C4-C5-N7	-3.55	106.52	110.58
2	O	202[B]	CMP	C4-C5-N7	-3.55	106.52	110.58
2	L	202[B]	CMP	C4-C5-N7	-3.55	106.53	110.58
2	O	201	CMP	C4-C5-N7	-3.51	106.57	110.58
2	I	201	CMP	O2P-P-O1P	3.48	119.26	108.56
2	F	201[B]	CMP	O2P-P-O1P	3.47	119.22	108.56
2	R	202[B]	CMP	N3-C2-N1	-3.45	123.35	128.58
2	Q	201	CMP	O5'-P-O3'	3.45	110.32	105.70
2	F	201[B]	CMP	C4-C5-N7	-3.44	106.65	110.58
2	O	201	CMP	N3-C2-N1	-3.43	123.39	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	201	CMP	N3-C2-N1	-3.43	123.39	128.58
2	Q	201	CMP	O2P-P-O1P	3.42	119.06	108.56
2	O	202[B]	CMP	N3-C2-N1	-3.42	123.41	128.58
2	H	201	CMP	O2P-P-O1P	3.40	119.01	108.56
2	R	201	CMP	O2P-P-O1P	3.39	118.98	108.56
2	O	202[B]	CMP	C4-N9-C8	3.36	109.27	105.74
2	B	201	CMP	O2P-P-O1P	3.35	118.86	108.56
2	F	201[A]	CMP	O2P-P-O1P	3.34	118.84	108.56
2	R	201	CMP	N3-C2-N1	-3.34	123.52	128.58
2	L	201	CMP	O2P-P-O1P	3.32	118.76	108.56
2	B	201	CMP	N3-C2-N1	-3.30	123.58	128.58
2	L	202[B]	CMP	N3-C2-N1	-3.29	123.59	128.58
2	O	201	CMP	O2P-P-O1P	3.29	118.67	108.56
2	A	201	CMP	O2P-P-O1P	3.28	118.63	108.56
2	M	201	CMP	N3-C2-N1	-3.26	123.64	128.58
2	R	202[B]	CMP	C4-N9-C8	3.26	109.16	105.74
2	E	201	CMP	O2P-P-O1P	3.22	118.47	108.56
2	A	201	CMP	N3-C2-N1	-3.22	123.71	128.58
2	L	201	CMP	N3-C2-N1	-3.21	123.73	128.58
2	R	202[A]	CMP	N3-C2-N1	-3.20	123.73	128.58
2	L	202[A]	CMP	N3-C2-N1	-3.19	123.75	128.58
2	M	201	CMP	O2P-P-O1P	3.19	118.35	108.56
2	B	202	CMP	C4-C5-N7	-3.16	106.97	110.58
2	I	201	CMP	N3-C2-N1	-3.15	123.81	128.58
2	Q	201	CMP	N3-C2-N1	-3.15	123.82	128.58
2	D	201[B]	CMP	O2P-P-O1P	3.12	118.14	108.56
2	O	202[A]	CMP	N3-C2-N1	-3.11	123.88	128.58
2	D	201[B]	CMP	N3-C2-N1	-3.10	123.89	128.58
2	F	201[A]	CMP	N3-C2-N1	-3.09	123.91	128.58
2	E	201	CMP	N3-C2-N1	-3.09	123.91	128.58
2	J	201	CMP	O2P-P-O1P	3.07	118.01	108.56
2	J	201	CMP	N3-C2-N1	-3.07	123.94	128.58
2	R	202[A]	CMP	O2P-P-O1P	3.06	117.96	108.56
2	D	201[A]	CMP	N3-C2-N1	-3.01	124.03	128.58
2	L	202[B]	CMP	C4-N9-C8	2.99	108.88	105.74
2	O	202[A]	CMP	O2P-P-O1P	2.99	117.74	108.56
2	B	202	CMP	O2P-P-O1P	2.95	117.63	108.56
2	G	201	CMP	O2P-P-O1P	2.95	117.62	108.56
2	G	201	CMP	N3-C2-N1	-2.93	124.14	128.58
2	D	201[A]	CMP	C4-C5-N7	-2.93	107.23	110.58
2	D	201[A]	CMP	O5'-P-O3'	2.90	109.58	105.70
2	F	201[B]	CMP	N3-C2-N1	-2.86	124.25	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	201	CMP	C4-N9-C8	2.83	108.71	105.74
2	M	201	CMP	C4-N9-C8	2.82	108.70	105.74
2	B	202	CMP	N3-C2-N1	-2.80	124.34	128.58
2	O	202[B]	CMP	O2P-P-O1P	2.79	117.14	108.56
2	M	201	CMP	C5-N7-C8	2.78	107.82	103.45
2	A	201	CMP	C4-N9-C8	2.76	108.64	105.74
2	Q	201	CMP	C5-N7-C8	2.76	107.79	103.45
2	O	202[B]	CMP	O5'-P-O3'	2.75	109.38	105.70
2	I	201	CMP	C4-N9-C8	2.74	108.62	105.74
2	A	201	CMP	C5-N7-C8	2.72	107.72	103.45
2	B	202	CMP	C1'-N9-C8	-2.71	121.09	127.09
2	E	201	CMP	C4-N9-C8	2.69	108.56	105.74
2	L	201	CMP	C5-N7-C8	2.68	107.66	103.45
2	E	201	CMP	C5-N7-C8	2.66	107.64	103.45
2	J	201	CMP	C5-N7-C8	2.64	107.60	103.45
2	F	201[B]	CMP	O5'-C5'-C4'	2.64	111.86	105.71
2	L	201	CMP	C4-N9-C8	2.62	108.49	105.74
2	D	201[B]	CMP	C5-N7-C8	2.62	107.57	103.45
2	I	201	CMP	C5-N7-C8	2.61	107.56	103.45
2	R	201	CMP	C5-N7-C8	2.61	107.55	103.45
2	R	202[A]	CMP	C5-N7-C8	2.60	107.54	103.45
2	O	202[A]	CMP	C5-N7-C8	2.59	107.52	103.45
2	R	201	CMP	C4-N9-C8	2.58	108.45	105.74
2	F	201[A]	CMP	C4-N9-C8	2.58	108.44	105.74
2	B	201	CMP	C5-N7-C8	2.56	107.47	103.45
2	L	202[A]	CMP	C5-N7-C8	2.55	107.46	103.45
2	F	201[A]	CMP	C5-N7-C8	2.55	107.45	103.45
2	M	201	CMP	C6-C5-N7	2.54	136.99	132.09
2	L	202[B]	CMP	O5'-P-O1P	-2.54	104.58	110.44
2	L	202[B]	CMP	C5-N7-C8	2.53	107.43	103.45
2	H	201	CMP	C4-N9-C8	2.53	108.40	105.74
2	H	201	CMP	C5-N7-C8	2.53	107.43	103.45
2	G	201	CMP	O5'-P-O3'	2.53	109.09	105.70
2	R	202[B]	CMP	C6-C5-N7	2.52	136.96	132.09
2	J	201	CMP	C4-N9-C8	2.52	108.38	105.74
2	L	202[A]	CMP	C4-N9-C8	2.52	108.38	105.74
2	G	201	CMP	C5-N7-C8	2.51	107.39	103.45
2	R	202[B]	CMP	C5-N7-C8	2.50	107.38	103.45
2	F	201[B]	CMP	O5'-P-O3'	2.50	109.05	105.70
2	A	201	CMP	O5'-C5'-C4'	2.47	111.46	105.71
2	D	201[A]	CMP	C4-N9-C8	2.46	108.32	105.74
2	A	201	CMP	C6-C5-N7	2.46	136.83	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	201	CMP	C5-N7-C8	2.45	107.30	103.45
2	O	202[B]	CMP	C6-C5-N7	2.42	136.76	132.09
2	O	202[B]	CMP	C5-N7-C8	2.41	107.24	103.45
2	R	202[B]	CMP	O5'-P-O3'	2.41	108.93	105.70
2	B	201	CMP	C4-N9-C8	2.41	108.27	105.74
2	R	202[A]	CMP	C4-N9-C8	2.41	108.26	105.74
2	M	201	CMP	O5'-C5'-C4'	2.39	111.28	105.71
2	B	202	CMP	O5'-P-O1P	-2.38	104.95	110.44
2	L	202[A]	CMP	C6-C5-N7	2.38	136.68	132.09
2	R	202[B]	CMP	N9-C8-N7	-2.36	110.59	113.94
2	R	202[A]	CMP	C6-C5-N7	2.36	136.63	132.09
2	L	202[B]	CMP	C6-C5-N7	2.35	136.61	132.09
2	F	201[A]	CMP	C6-C5-N7	2.34	136.61	132.09
2	F	201[B]	CMP	O5'-P-O1P	-2.34	105.04	110.44
2	F	201[B]	CMP	C5-N7-C8	2.34	107.12	103.45
2	O	202[A]	CMP	C4-N9-C8	2.33	108.19	105.74
2	Q	201	CMP	O3'-P-O1P	-2.32	105.42	110.39
2	Q	201	CMP	C6-C5-N7	2.31	136.53	132.09
2	J	201	CMP	C6-C5-N7	2.30	136.53	132.09
2	O	202[A]	CMP	C6-C5-N7	2.28	136.50	132.09
2	D	201[B]	CMP	C4-N9-C8	2.28	108.14	105.74
2	M	201	CMP	O3'-P-O1P	-2.28	105.50	110.39
2	D	201[B]	CMP	C6-C5-N7	2.27	136.47	132.09
2	O	201	CMP	C4-N9-C8	2.27	108.12	105.74
2	G	201	CMP	C6-C5-N7	2.26	136.45	132.09
2	I	201	CMP	C6-C5-N7	2.26	136.45	132.09
2	Q	201	CMP	O5'-C5'-C4'	2.26	110.97	105.71
2	H	201	CMP	C6-C5-N7	2.25	136.44	132.09
2	O	202[B]	CMP	O3'-P-O1P	-2.25	105.56	110.39
2	J	201	CMP	O5'-P-O3'	2.21	108.66	105.70
2	M	201	CMP	N9-C8-N7	-2.20	110.82	113.94
2	A	201	CMP	N9-C8-N7	-2.19	110.83	113.94
2	L	202[B]	CMP	N9-C8-N7	-2.18	110.85	113.94
2	R	201	CMP	C6-C5-N7	2.17	136.28	132.09
2	Q	201	CMP	N9-C8-N7	-2.16	110.87	113.94
2	O	202[B]	CMP	N9-C8-N7	-2.16	110.87	113.94
2	O	201	CMP	C6-C5-N7	2.16	136.25	132.09
2	L	201	CMP	C6-C5-N7	2.15	136.24	132.09
2	R	202[A]	CMP	O5'-P-O3'	2.15	108.58	105.70
2	L	202[B]	CMP	O3'-P-O1P	-2.12	105.84	110.39
2	B	202	CMP	O4'-C1'-N9	2.11	112.15	108.09
2	B	201	CMP	C6-C5-N7	2.11	136.15	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	202	CMP	C5-N7-C8	2.10	106.75	103.45
2	A	201	CMP	O3'-P-O1P	-2.10	105.89	110.39
2	E	201	CMP	C6-C5-N7	2.09	136.13	132.09
2	I	201	CMP	N9-C8-N7	-2.09	110.97	113.94
2	R	201	CMP	N9-C8-N7	-2.08	110.98	113.94
2	B	202	CMP	C4-N9-C1'	2.08	131.49	126.63
2	F	201[B]	CMP	C1'-N9-C8	-2.07	122.49	127.09
2	H	201	CMP	C2-N1-C6	2.07	122.12	118.73
2	L	201	CMP	N9-C8-N7	-2.06	111.02	113.94
2	F	201[B]	CMP	O3'-P-O1P	-2.06	105.98	110.39
2	E	201	CMP	N9-C8-N7	-2.04	111.03	113.94
2	F	201[A]	CMP	O5'-P-O1P	-2.04	105.74	110.44
2	L	202[A]	CMP	O5'-P-O1P	-2.02	105.79	110.44
2	D	201[A]	CMP	C5-N7-C8	2.01	106.61	103.45
2	F	201[A]	CMP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201[A]	CMP	C2'-C1'-N9-C8
2	F	201[B]	CMP	C2'-C1'-N9-C8
2	B	202	CMP	O4'-C1'-N9-C4
2	D	201[A]	CMP	C2'-C1'-N9-C4
2	F	201[B]	CMP	C2'-C1'-N9-C4
2	B	202	CMP	O4'-C1'-N9-C8
2	R	202[B]	CMP	C2'-C1'-N9-C8
2	R	202[B]	CMP	O4'-C1'-N9-C8

There are no ring outliers.

25 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	201	CMP	1	0
2	A	201	CMP	1	0
2	L	202[B]	CMP	3	0
2	M	201	CMP	1	0
2	H	201	CMP	1	0
4	R	203	SO4	1	0
2	B	201	CMP	1	0
2	O	202[A]	CMP	1	0

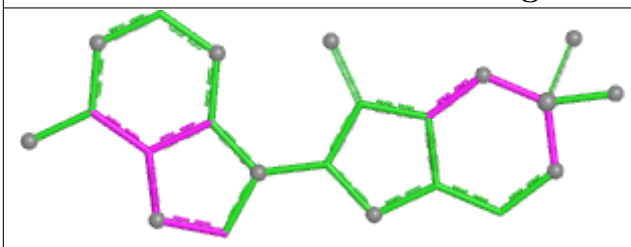
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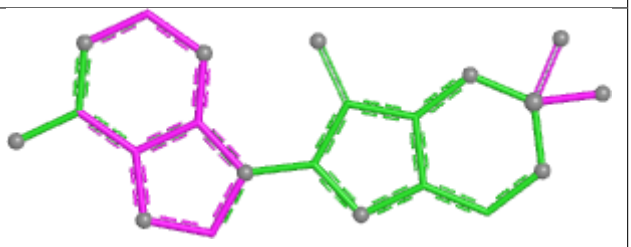
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201[A]	CMP	7	0
2	F	201[A]	CMP	1	0
2	B	202	CMP	2	0
2	R	201	CMP	1	0
2	G	201	CMP	2	0
2	R	202[A]	CMP	1	0
2	O	202[B]	CMP	3	0
2	D	201[B]	CMP	1	0
2	O	201	CMP	1	0
2	L	202[A]	CMP	1	0
2	E	201	CMP	1	0
2	I	201	CMP	2	0
2	Q	201	CMP	2	0
2	F	201[B]	CMP	4	0
4	O	203	SO4	1	0
2	J	201	CMP	1	0
2	R	202[B]	CMP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

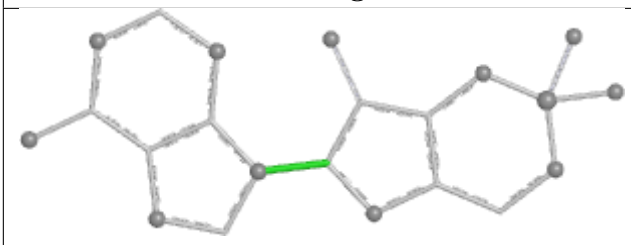
Ligand CMP L 201



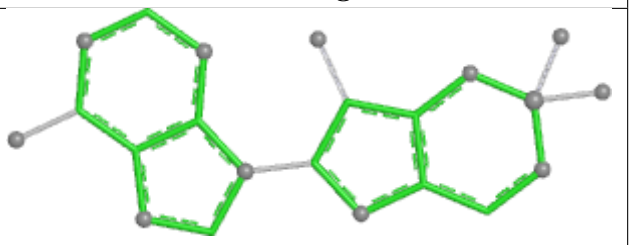
Bond lengths



Bond angles

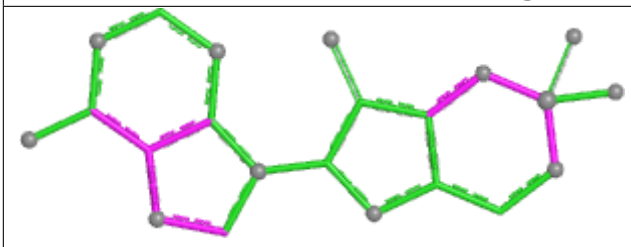


Torsions

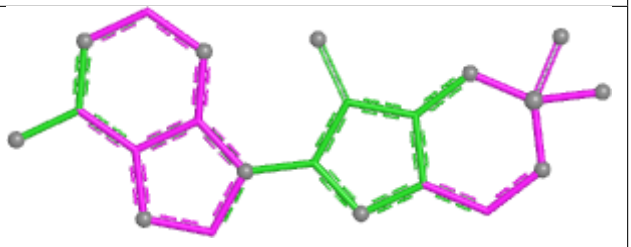


Rings

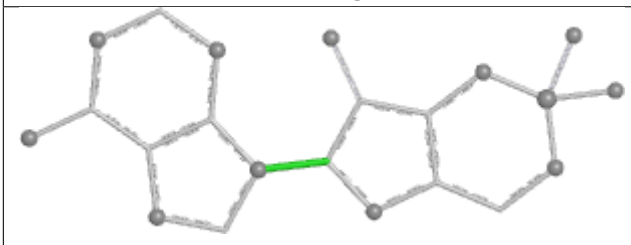
Ligand CMP A 201



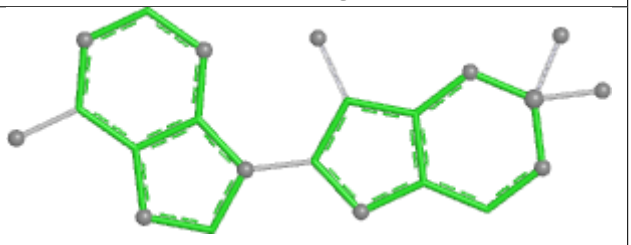
Bond lengths



Bond angles

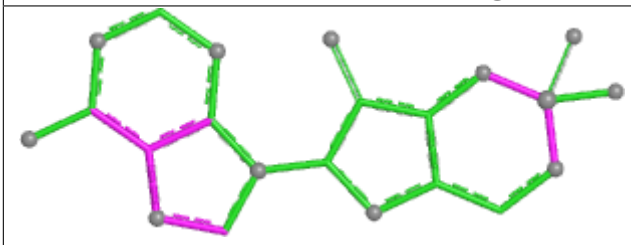


Torsions

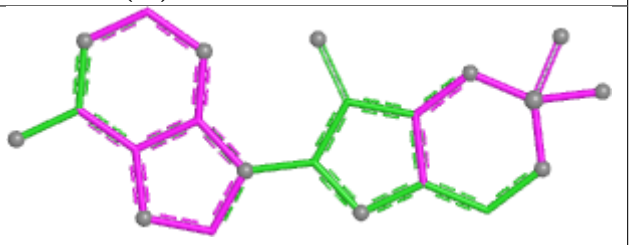


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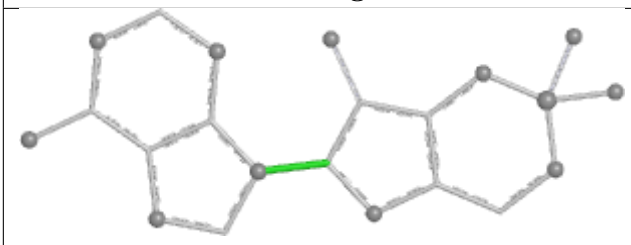
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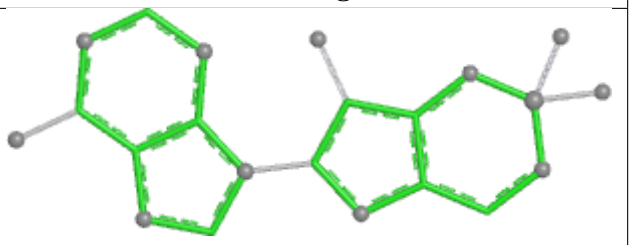
Bond lengths



Bond angles

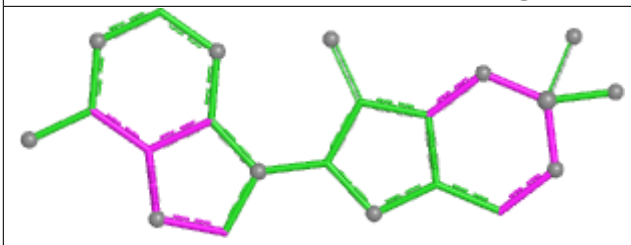


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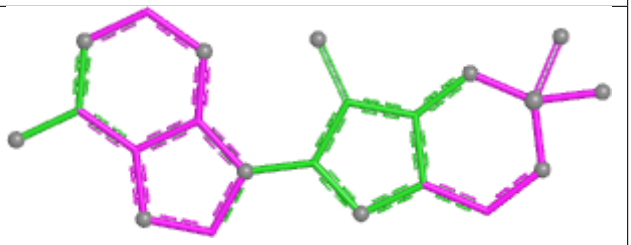


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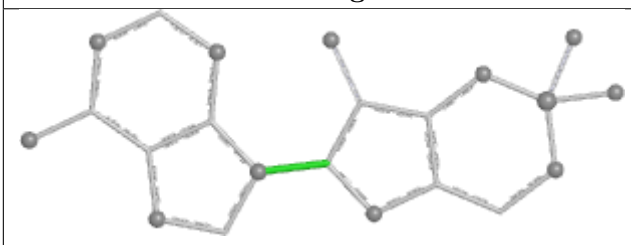
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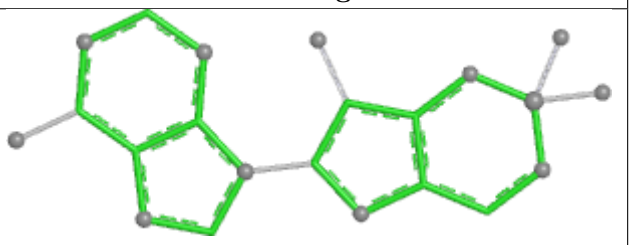
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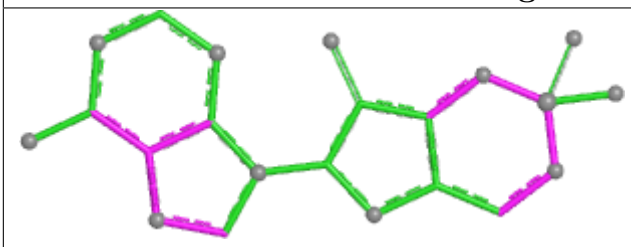


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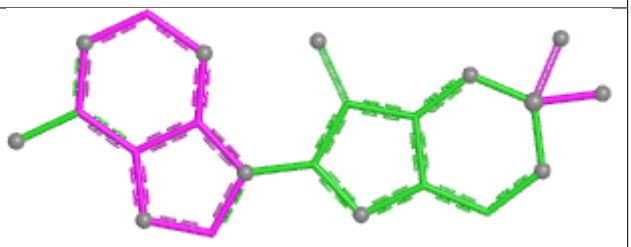


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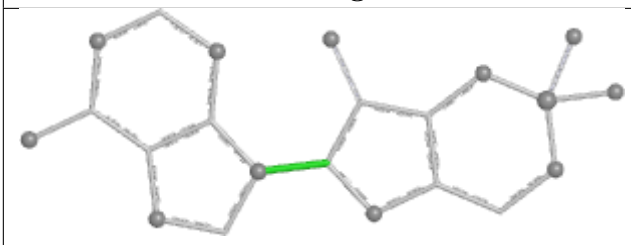
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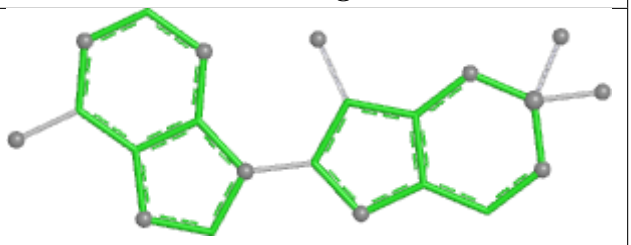
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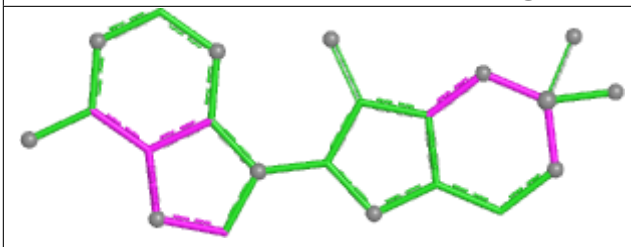


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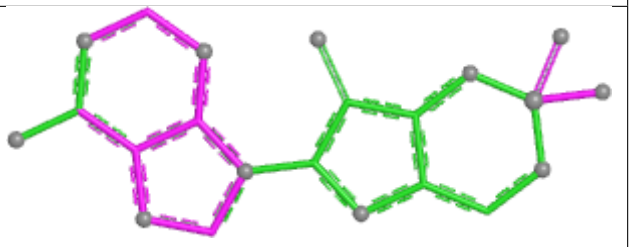


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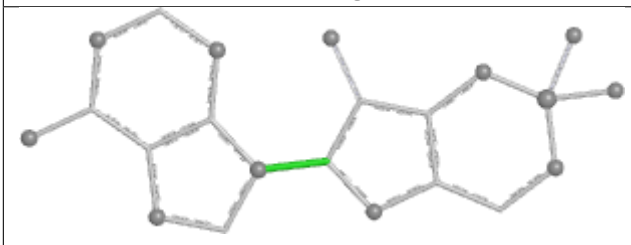
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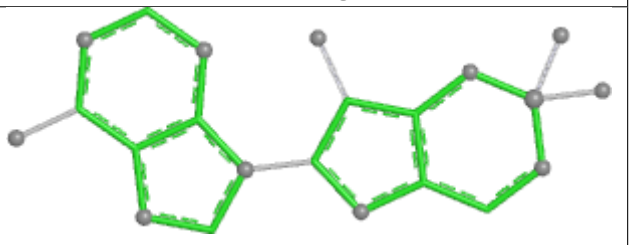
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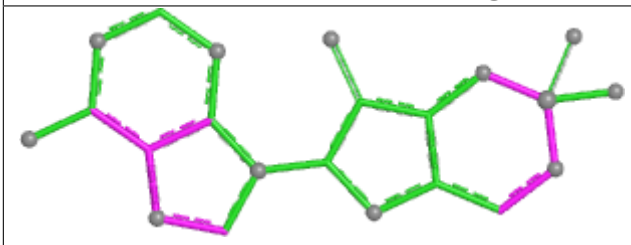


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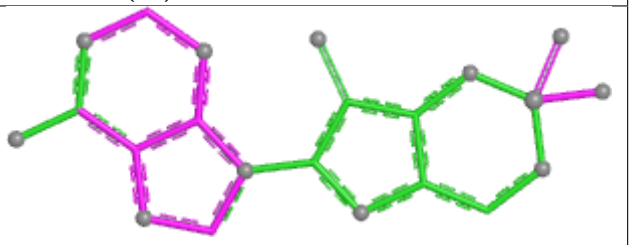


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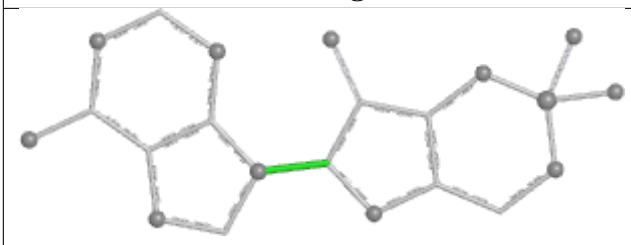
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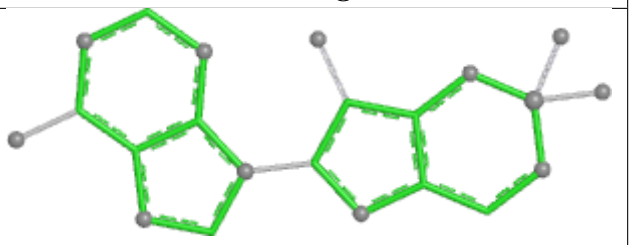
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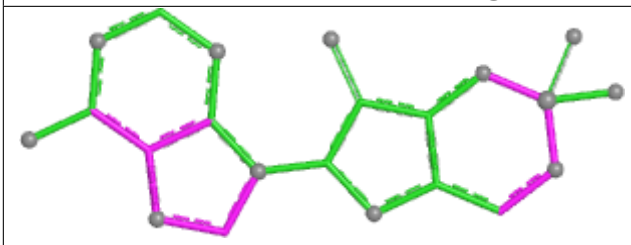


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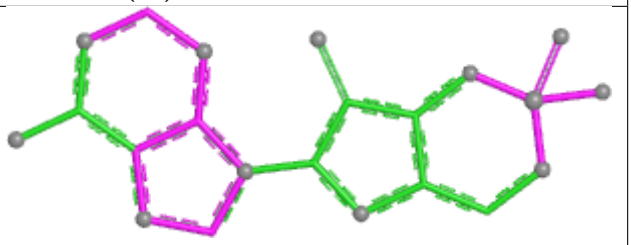


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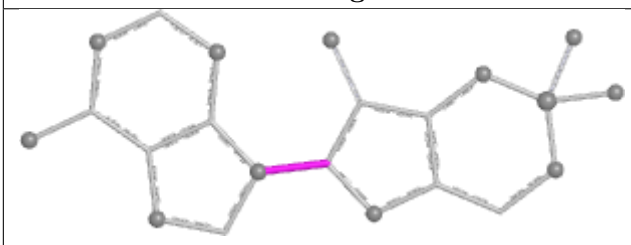
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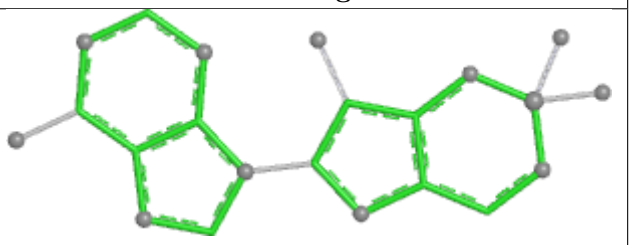
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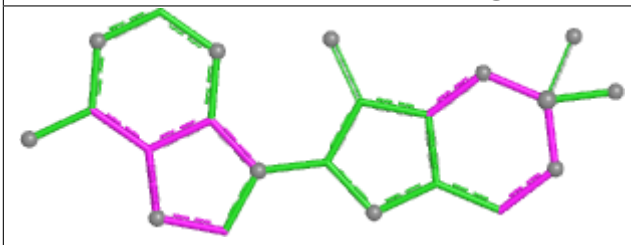


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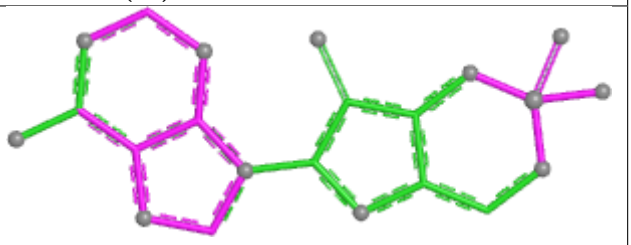


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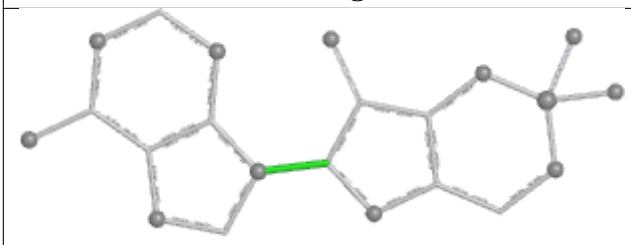
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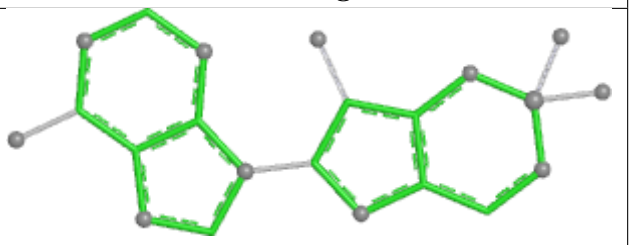
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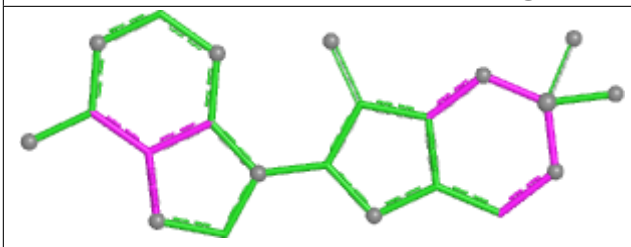


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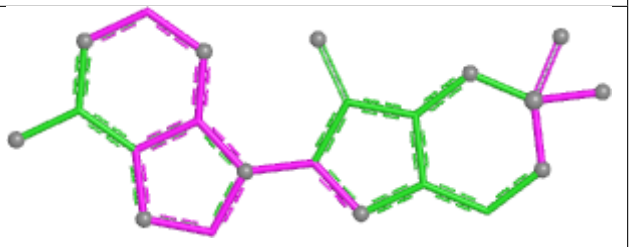


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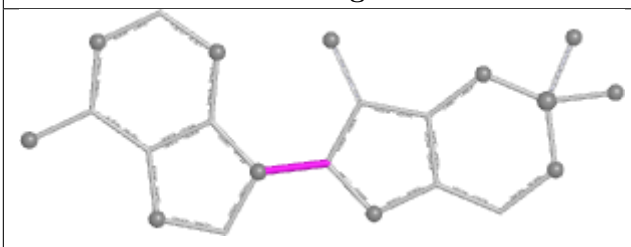
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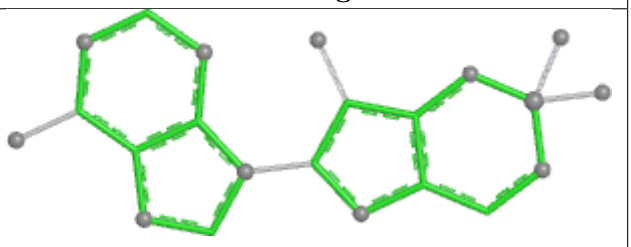
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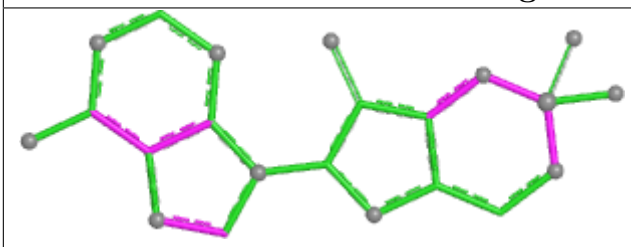


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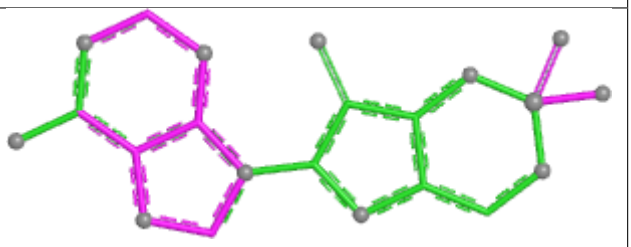


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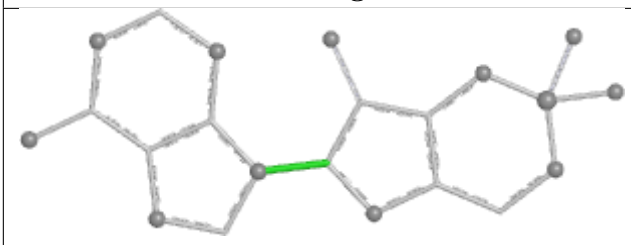
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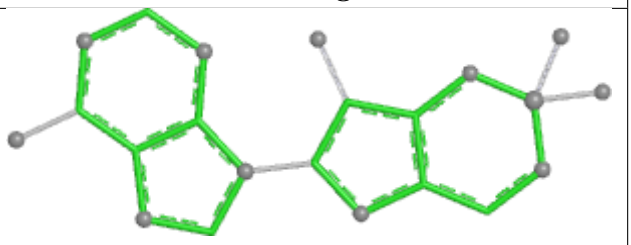
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Bond angles

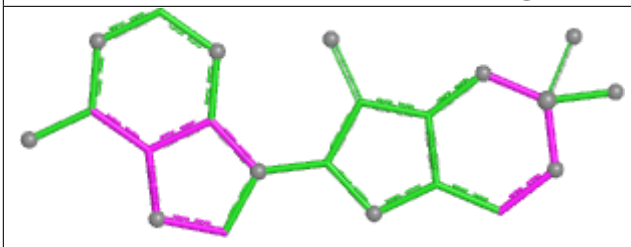


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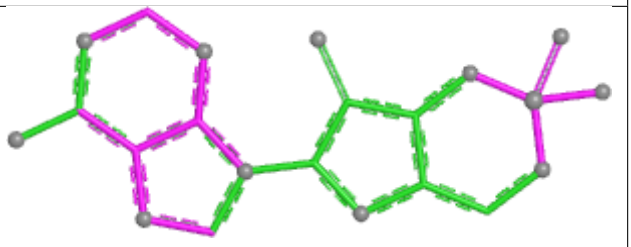


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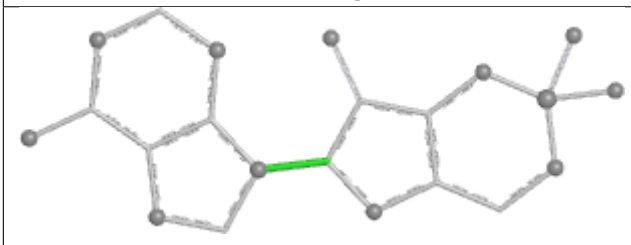
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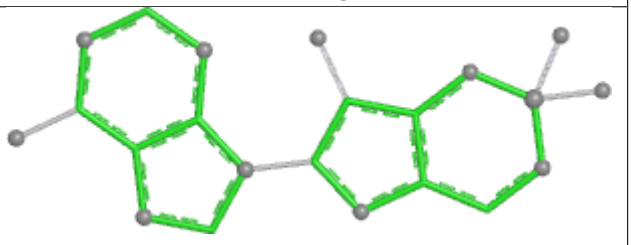
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Bond angles

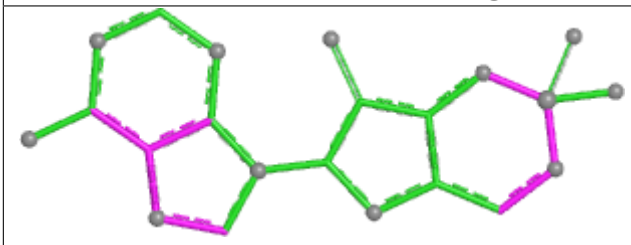


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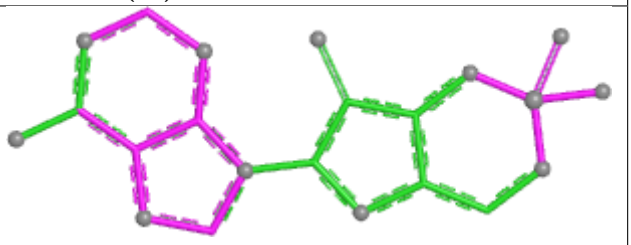


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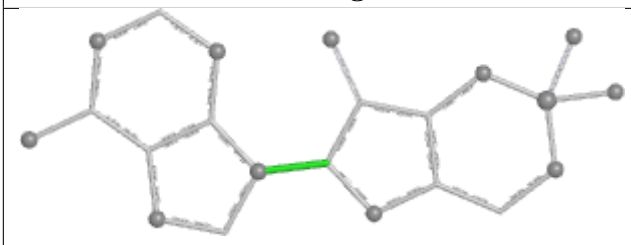
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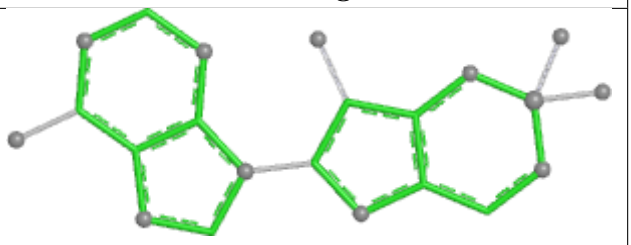
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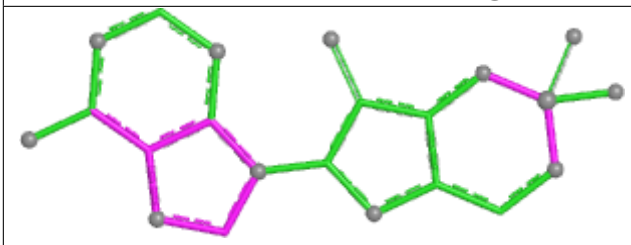


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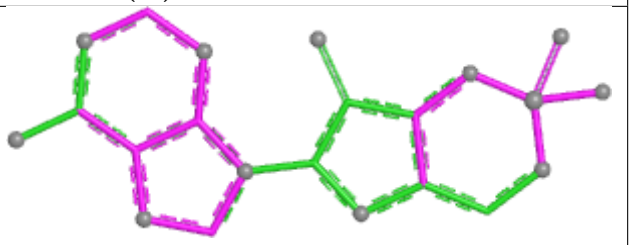


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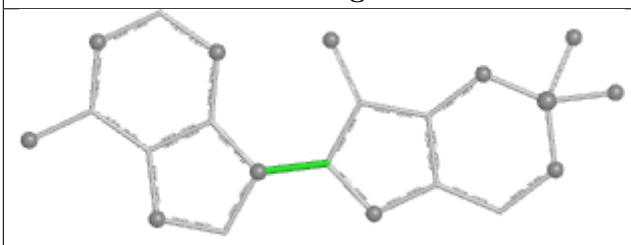
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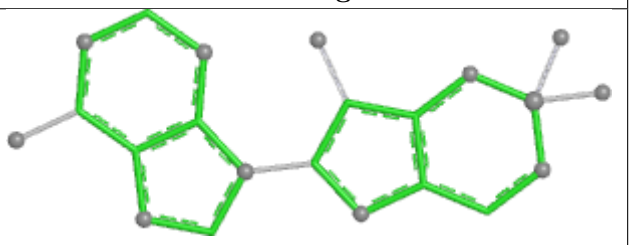
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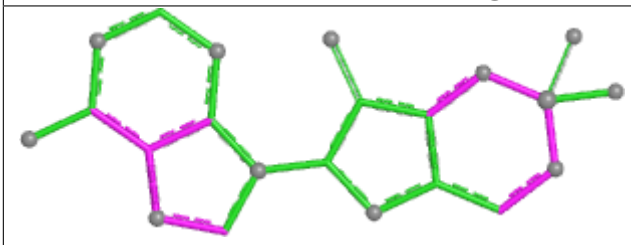


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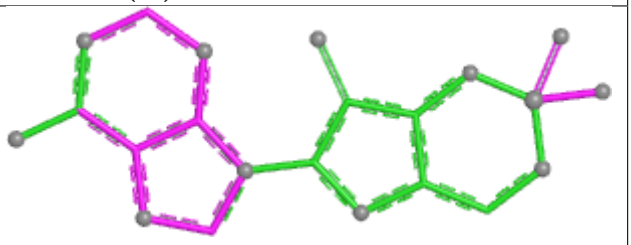


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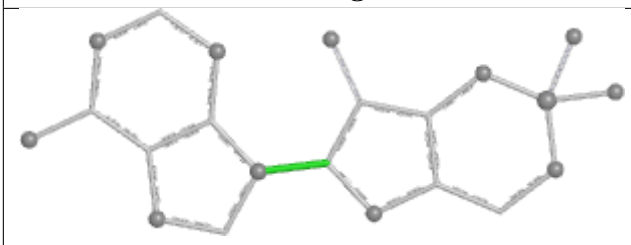
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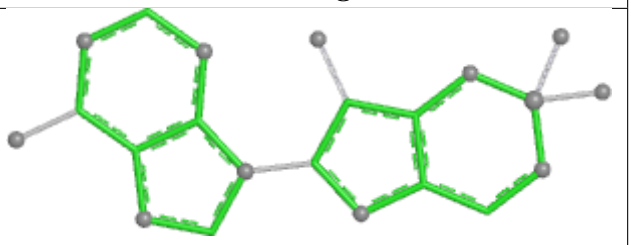
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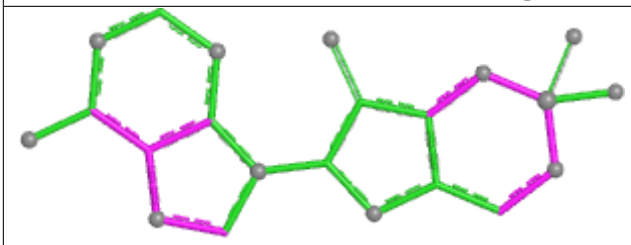


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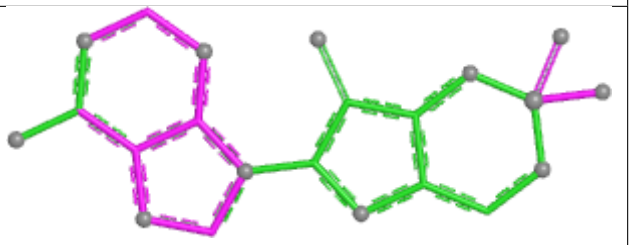


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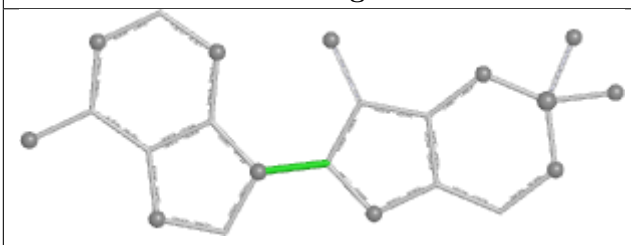
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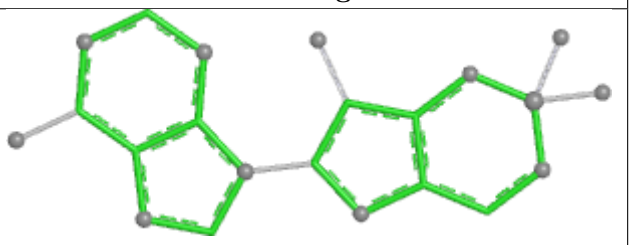
Bond lengths



Bond angles

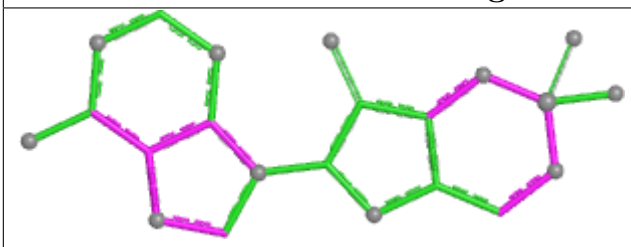


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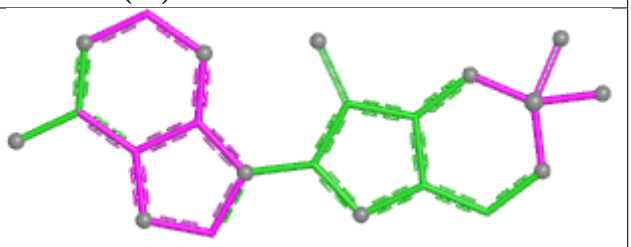


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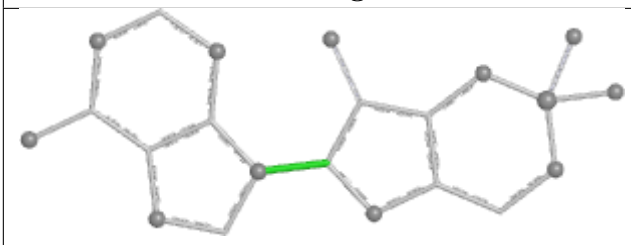
Ligand CMP L 202 (A)



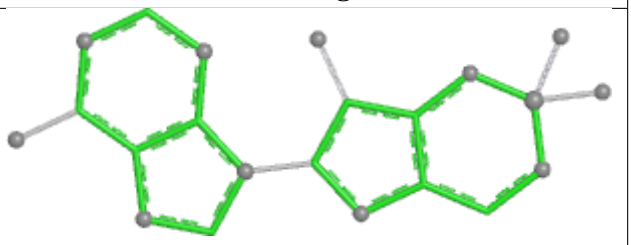
Bond lengths



Bond angles

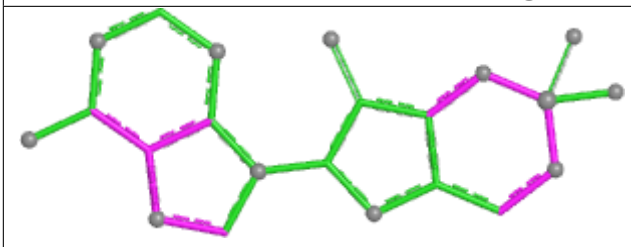


Torsions

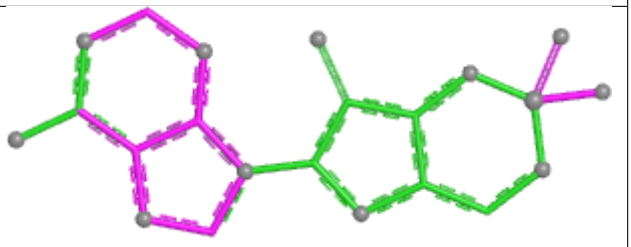


Rings

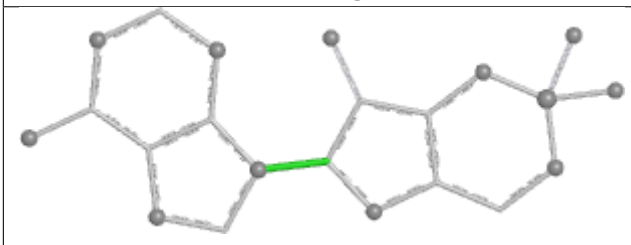
Ligand CMP E 201



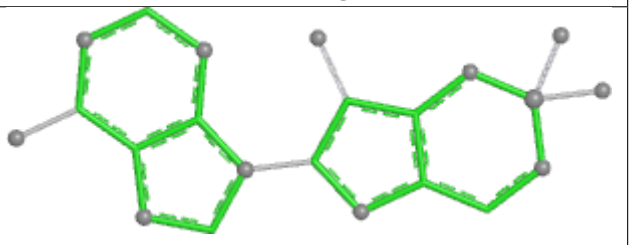
Bond lengths



Bond angles

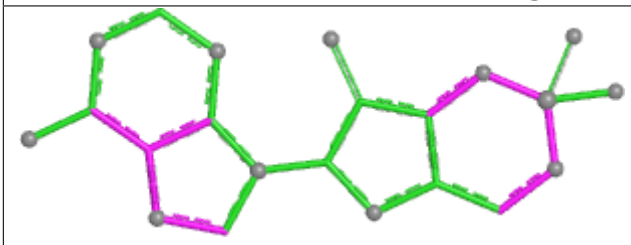


Torsions

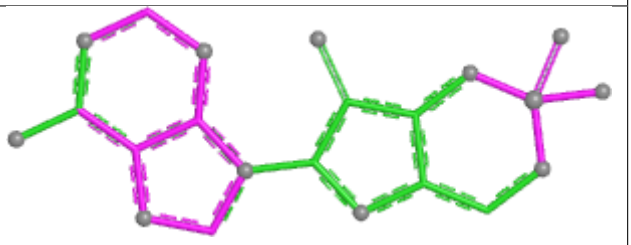


Rings

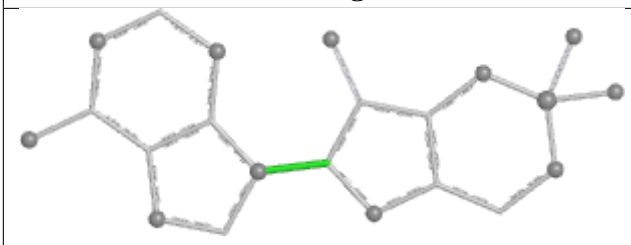
Ligand CMP I 201



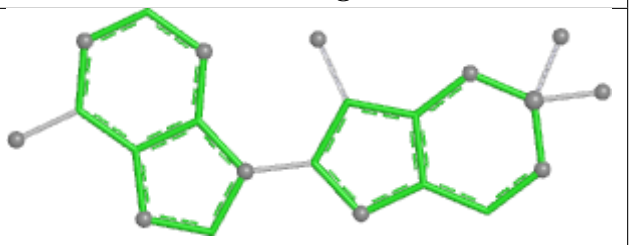
Bond lengths



Bond angles

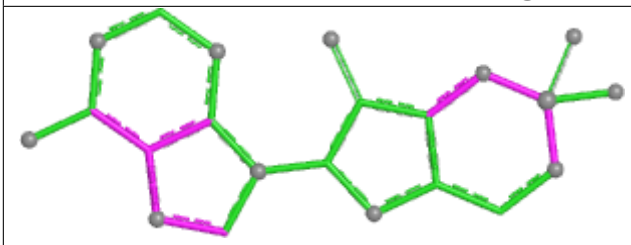


Torsions

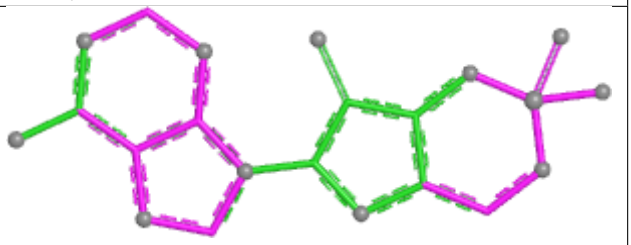


Rings

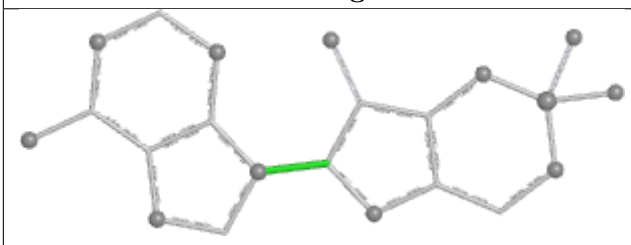
Ligand CMP Q 201



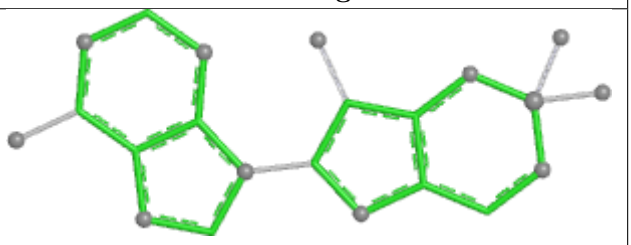
Bond lengths



Bond angles

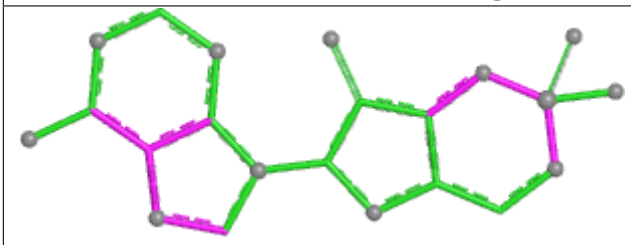


Torsions

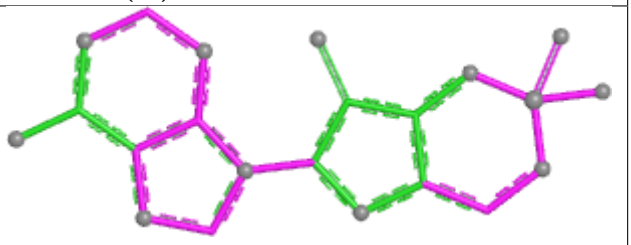


Rings

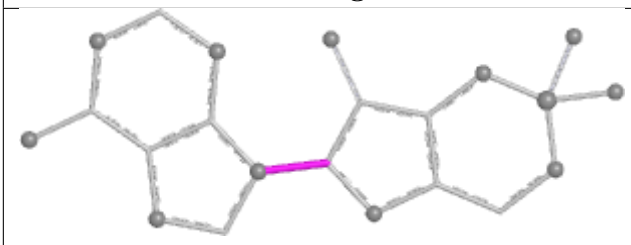
Ligand CMP F 201 (B)



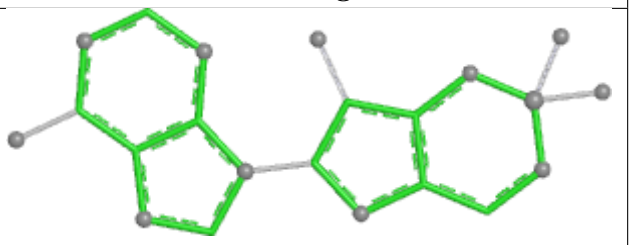
Bond lengths



Bond angles

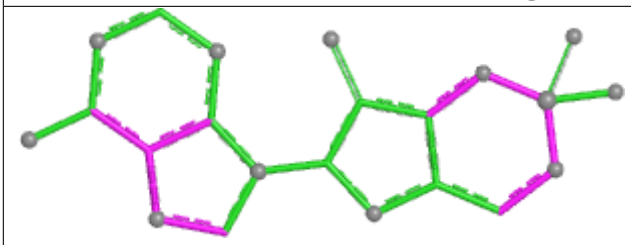


Torsions

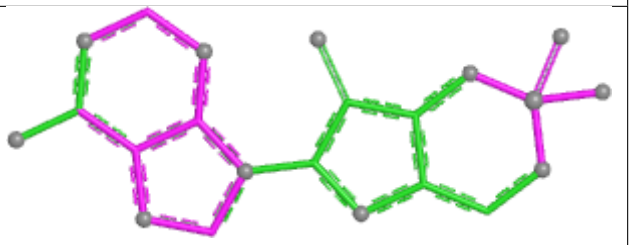


Rings

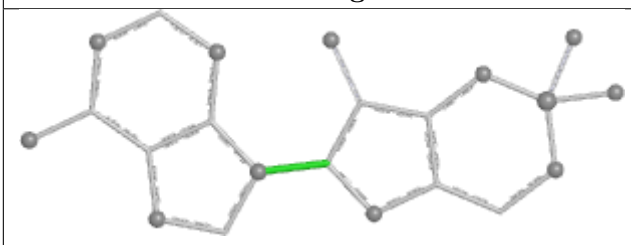
Ligand CMP J 201



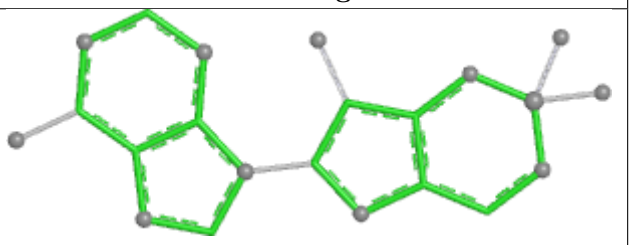
Bond lengths



Bond angles

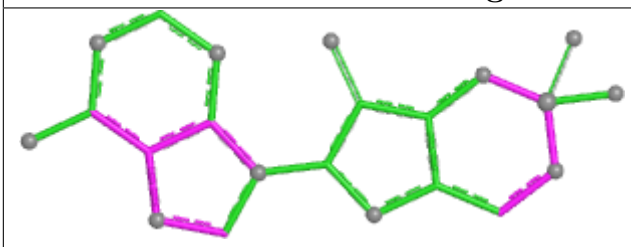


Torsions

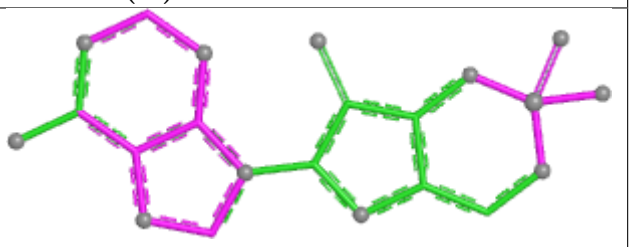


Rings

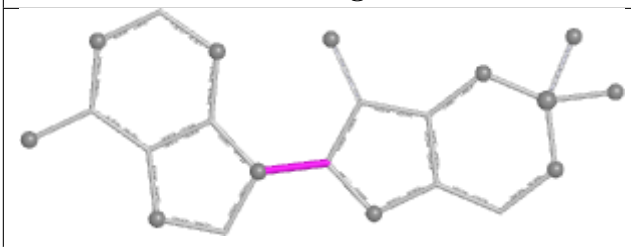
Ligand CMP R 202 (B)



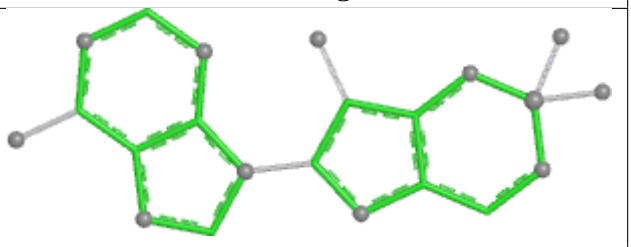
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	105/122 (86%)	-0.40	0	100	100	31, 67, 94, 101	0
1	B	108/122 (88%)	-0.59	0	100	100	27, 51, 76, 92	0
1	C	100/122 (81%)	-0.67	0	100	100	26, 44, 69, 87	0
1	D	101/122 (82%)	-0.62	0	100	100	27, 43, 72, 88	1 (0%)
1	E	103/122 (84%)	-0.49	0	100	100	31, 68, 96, 101	0
1	F	107/122 (87%)	-0.56	0	100	100	28, 51, 77, 87	3 (2%)
1	G	103/122 (84%)	-0.39	0	100	100	30, 68, 96, 104	0
1	H	106/122 (86%)	-0.52	0	100	100	27, 52, 80, 87	1 (0%)
1	I	100/122 (81%)	-0.68	0	100	100	26, 42, 70, 86	0
1	J	100/122 (81%)	-0.64	0	100	100	27, 44, 72, 91	1 (1%)
1	K	101/122 (82%)	-0.45	0	100	100	33, 66, 95, 100	0
1	L	108/122 (88%)	-0.61	0	100	100	30, 54, 78, 91	2 (1%)
1	M	100/122 (81%)	-0.68	0	100	100	26, 44, 71, 94	1 (1%)
1	N	101/122 (82%)	-0.39	0	100	100	32, 65, 95, 104	0
1	O	106/122 (86%)	-0.62	0	100	100	31, 52, 76, 88	0
1	P	100/122 (81%)	-0.58	0	100	100	29, 42, 70, 90	2 (2%)
1	Q	102/122 (83%)	-0.43	0	100	100	32, 68, 95, 103	0
1	R	108/122 (88%)	-0.52	0	100	100	29, 54, 78, 85	1 (0%)
All	All	1859/2196 (84%)	-0.55	0	100	100	26, 53, 90, 104	12 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	203	1/1	0.96	0.06	54,54,54,54	0
3	MG	G	202	1/1	0.96	0.04	61,61,61,61	0
2	CMP	R	202[A]	22/22	0.97	0.06	47,52,62,68	22
2	CMP	R	202[B]	22/22	0.97	0.06	46,53,62,68	22
3	MG	K	201	1/1	0.97	0.04	62,62,62,62	0
3	MG	P	201	1/1	0.97	0.06	56,56,56,56	0
2	CMP	M	201	22/22	0.98	0.04	44,50,56,62	0
2	CMP	O	201	22/22	0.98	0.04	26,32,38,39	0
2	CMP	O	202[A]	22/22	0.98	0.05	49,54,63,74	22
2	CMP	O	202[B]	22/22	0.98	0.05	49,55,66,74	22
2	CMP	Q	201	22/22	0.98	0.04	29,43,55,57	0
2	CMP	F	201[A]	22/22	0.98	0.05	51,56,68,76	22
2	CMP	F	201[B]	22/22	0.98	0.05	51,57,68,76	22
2	CMP	A	201	22/22	0.98	0.04	37,45,50,54	0
2	CMP	I	201	22/22	0.98	0.05	48,54,62,70	0
2	CMP	L	202[A]	22/22	0.98	0.05	49,54,66,78	22
3	MG	N	201	1/1	0.98	0.05	60,60,60,60	0
2	CMP	L	202[B]	22/22	0.98	0.05	49,56,69,78	22
2	CMP	G	201	22/22	0.99	0.04	46,57,64,74	0
2	CMP	H	201	22/22	0.99	0.03	24,30,38,41	0
2	CMP	R	201	22/22	0.99	0.03	22,29,37,37	0
2	CMP	J	201	22/22	0.99	0.04	41,53,60,68	0
2	CMP	L	201	22/22	0.99	0.04	27,31,37,39	0
3	MG	E	202	1/1	0.99	0.03	56,56,56,56	0
2	CMP	D	201[B]	22/22	0.99	0.05	37,45,66,82	22
2	CMP	E	201	22/22	0.99	0.04	39,48,54,57	0
2	CMP	B	201	22/22	0.99	0.04	24,32,36,39	0
2	CMP	B	202	22/22	0.99	0.04	36,46,57,61	0
2	CMP	D	201[A]	22/22	0.99	0.05	37,47,67,82	22
4	SO4	F	202	5/5	0.99	0.03	54,55,57,59	0
4	SO4	B	204	5/5	0.99	0.03	49,53,55,60	0
4	SO4	G	203	5/5	0.99	0.04	47,50,56,63	0

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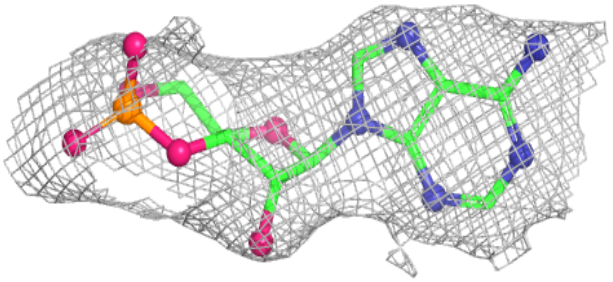
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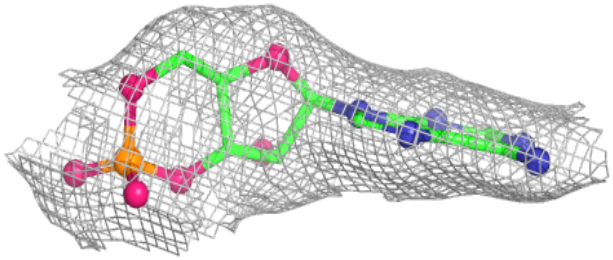
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	J	202	5/5	0.99	0.03	56,60,61,63	0
4	SO4	O	203	5/5	0.99	0.03	56,56,61,63	0
4	SO4	R	203	5/5	0.99	0.03	51,58,59,62	0

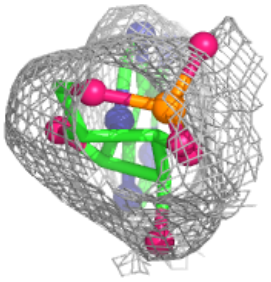
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CMP R 202 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

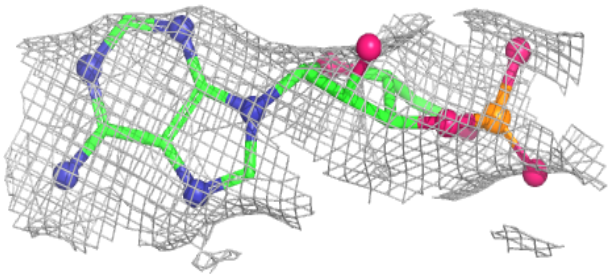


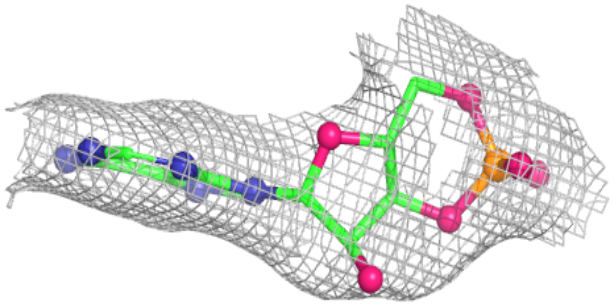


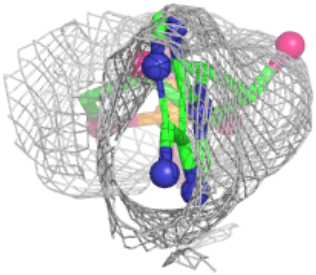


Electron density around CMP R 202 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

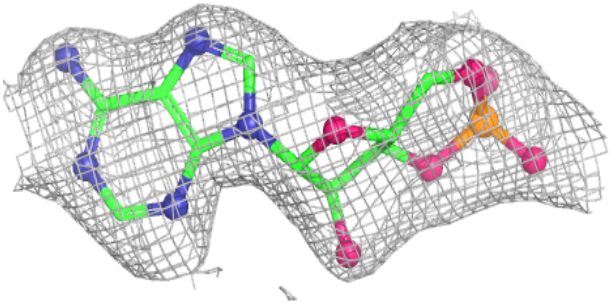


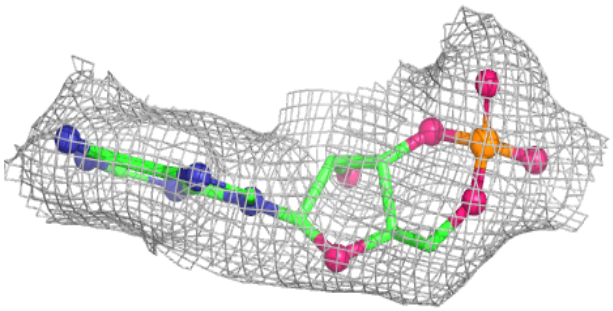


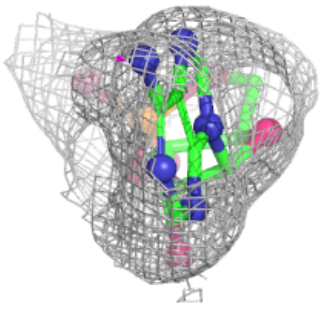


Electron density around CMP M 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

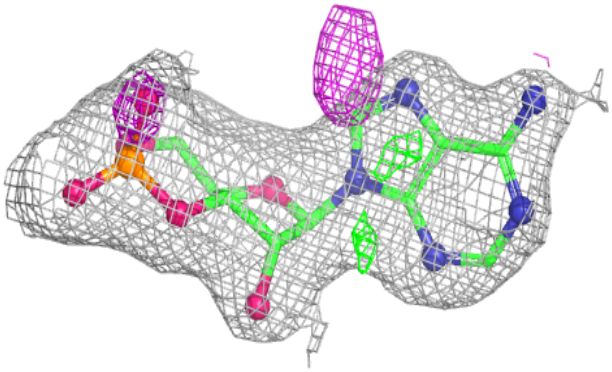


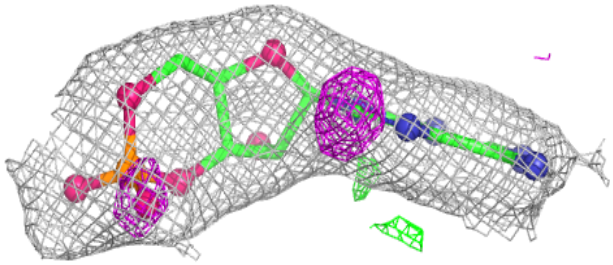


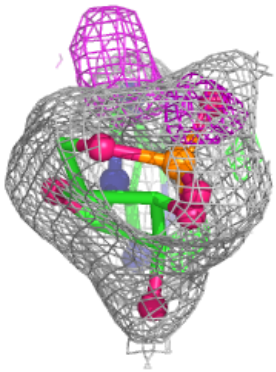


Electron density around CMP O 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

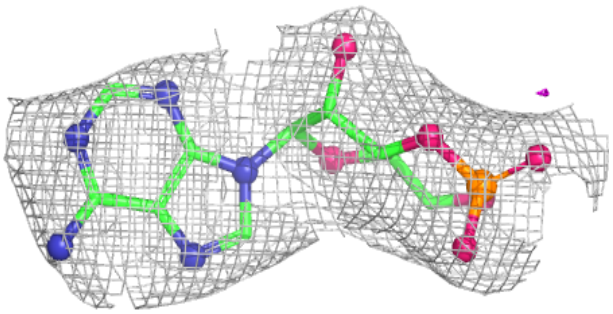


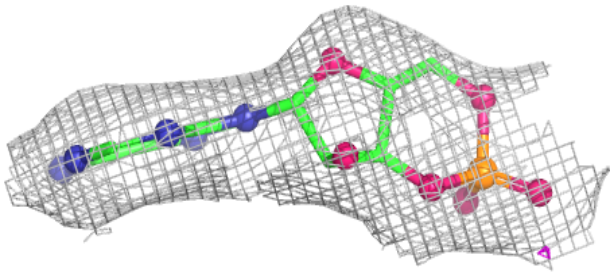


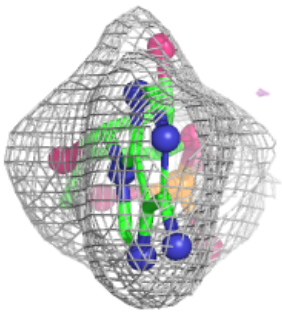


Electron density around CMP O 202 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

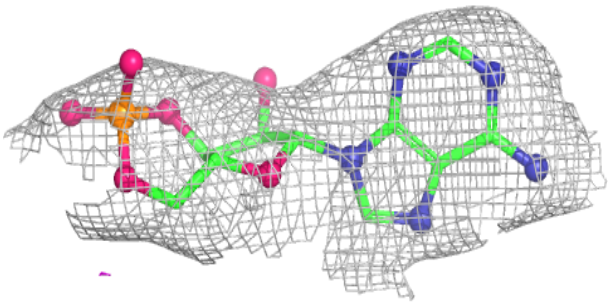


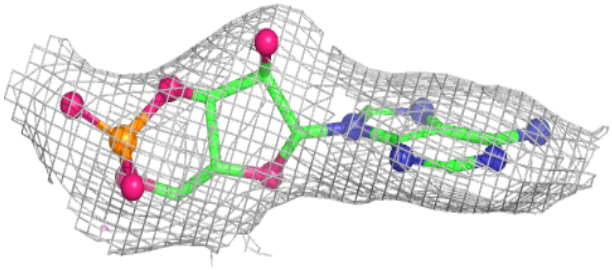


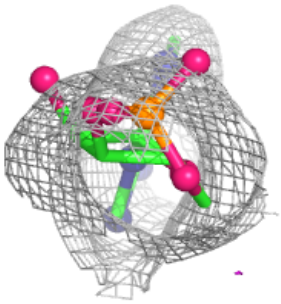


Electron density around CMP O 202 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

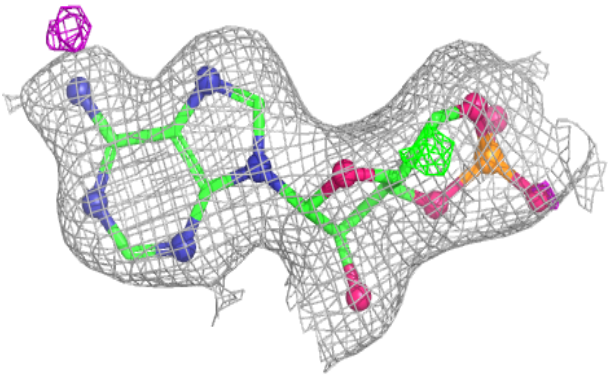


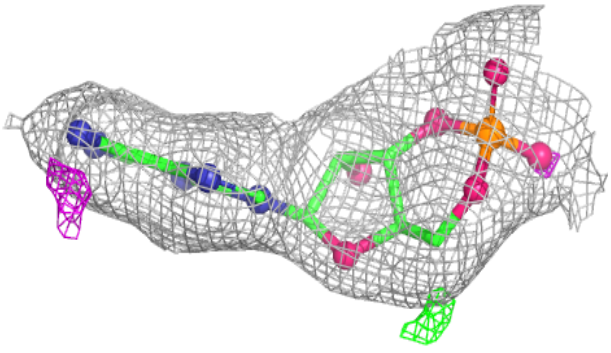


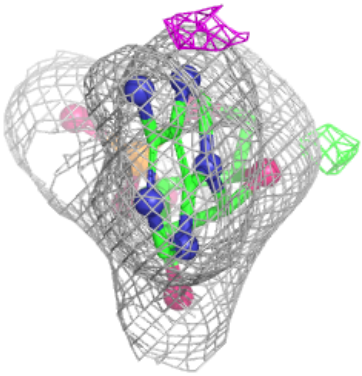


Electron density around CMP Q 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

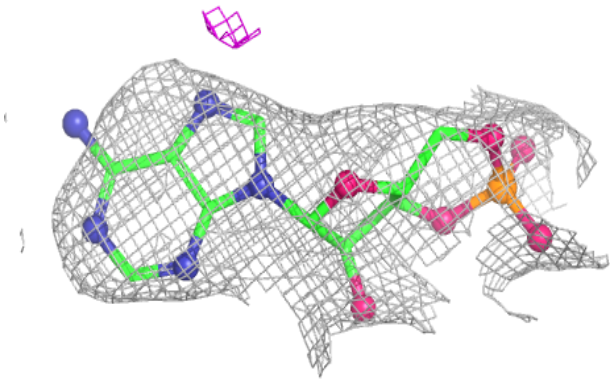


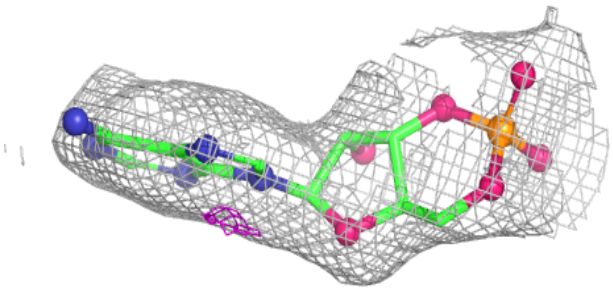


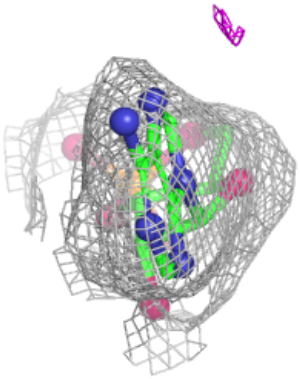


Electron density around CMP F 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

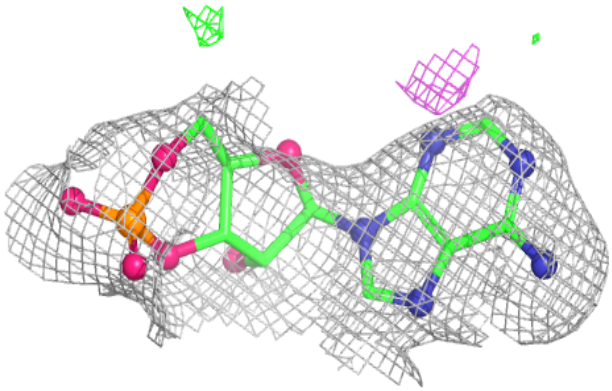


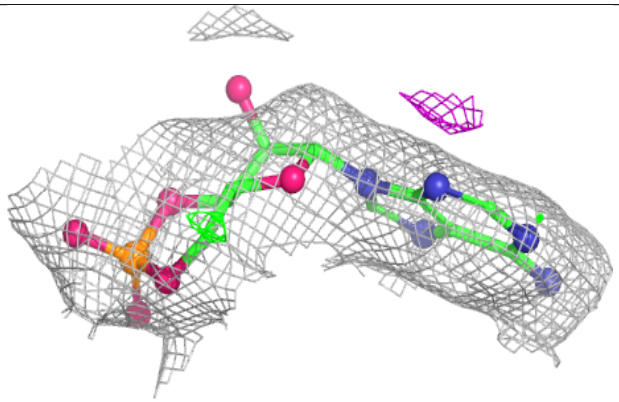


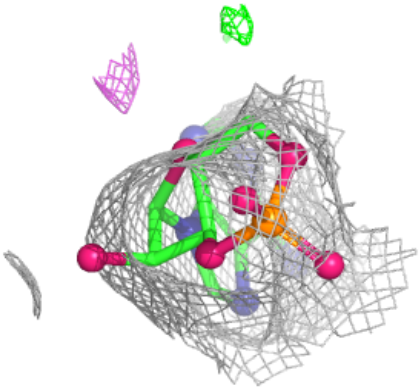


Electron density around CMP F 201 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

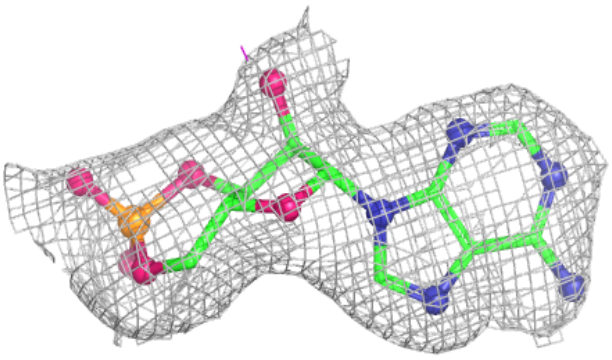


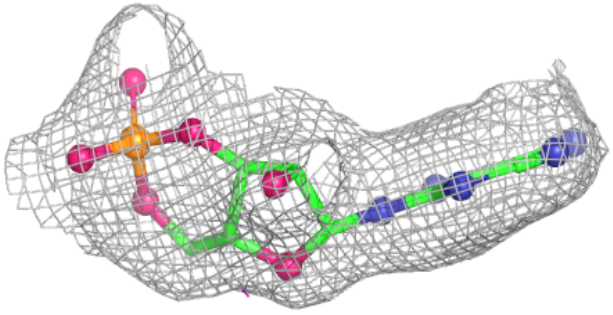


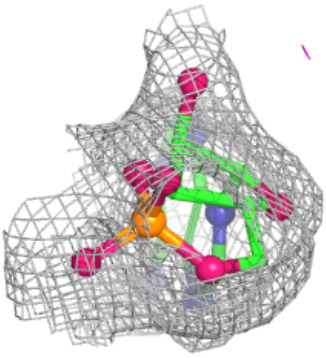


Electron density around CMP A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

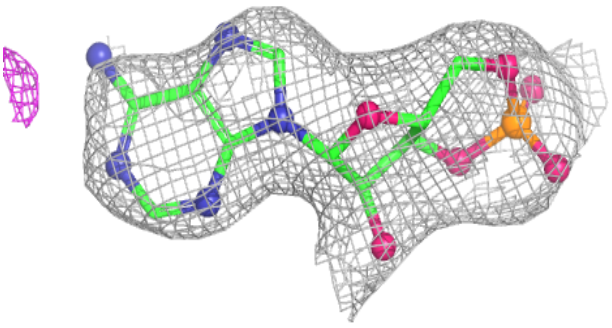


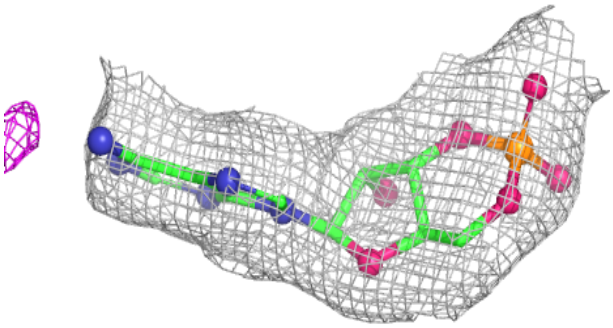


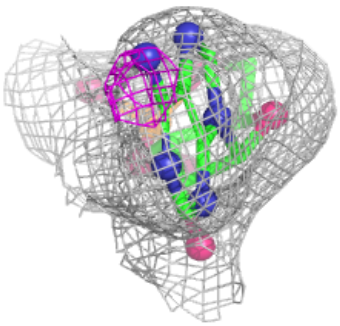


Electron density around CMP I 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

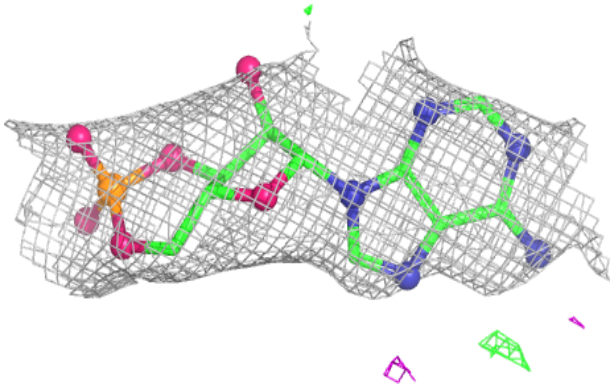


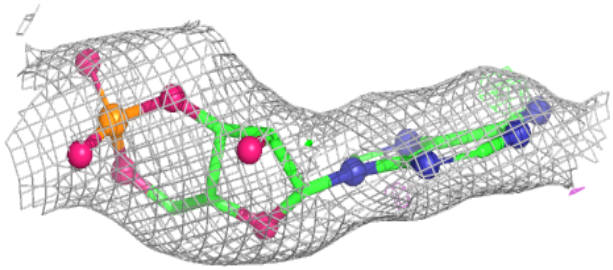


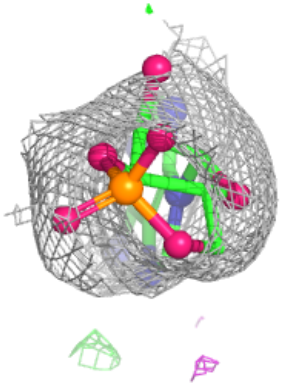


Electron density around CMP L 202 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

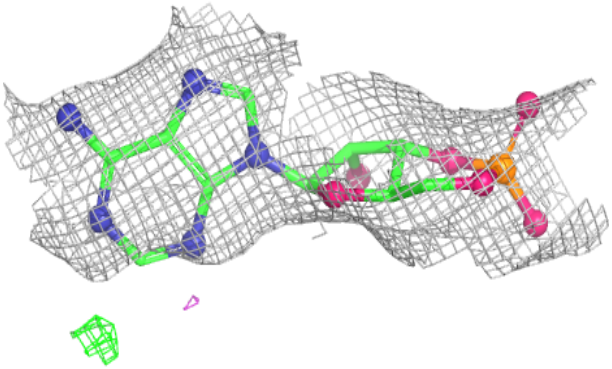


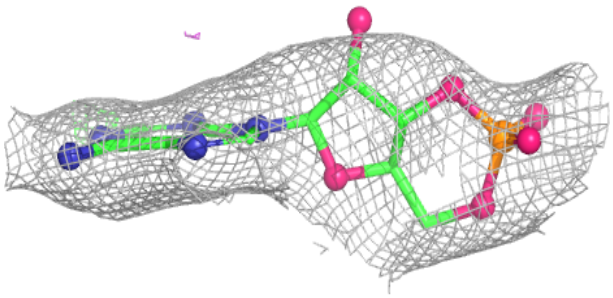


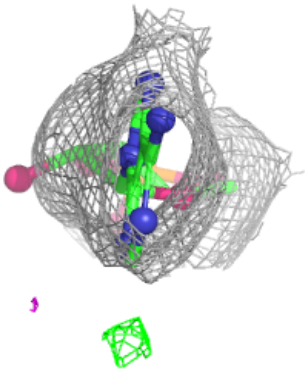


Electron density around CMP L 202 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

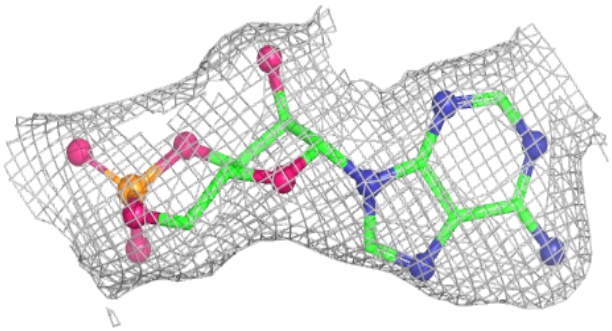


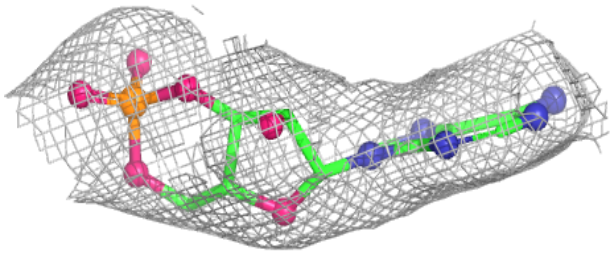


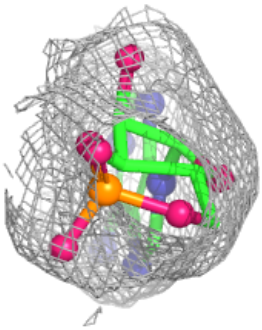


Electron density around CMP G 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

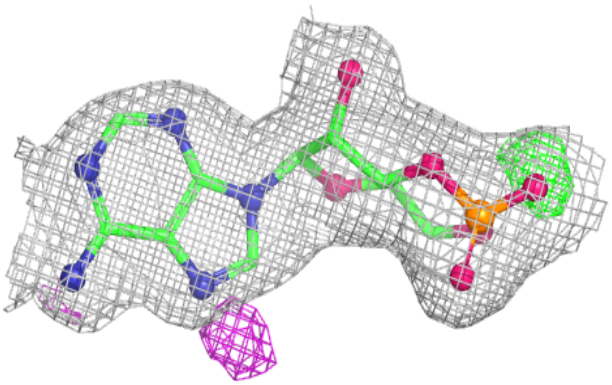


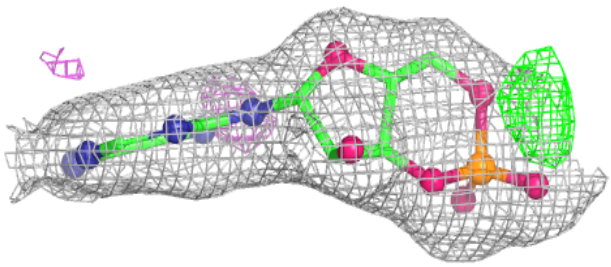


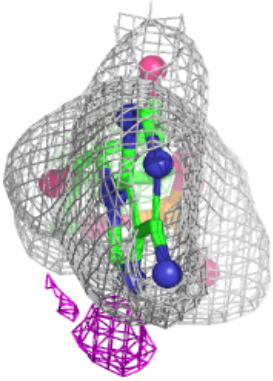


Electron density around CMP H 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

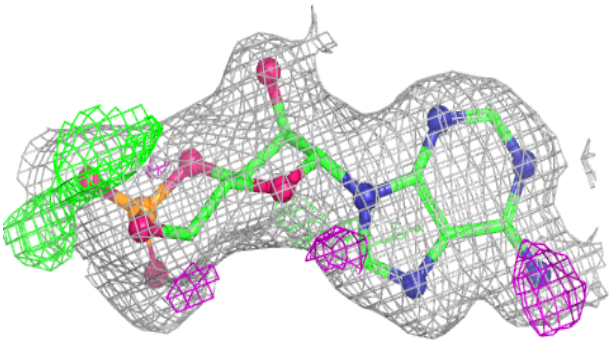


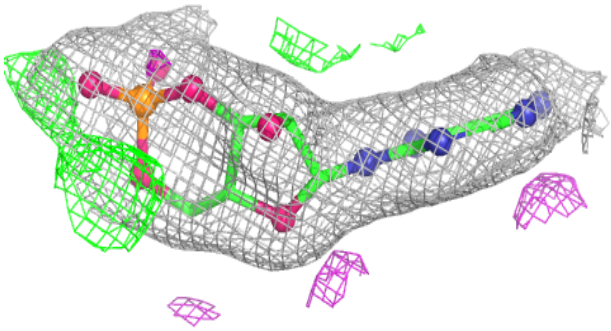


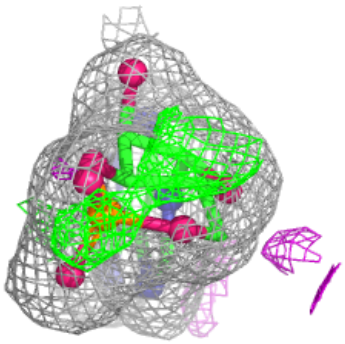


Electron density around CMP R 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

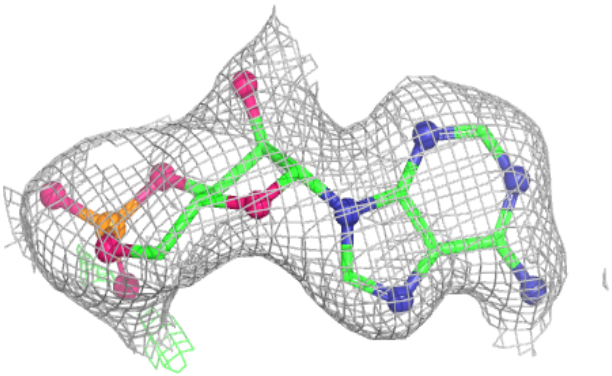


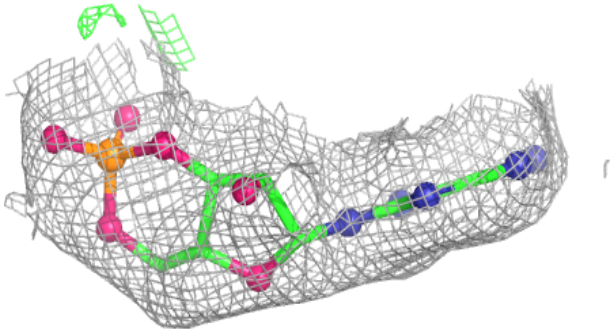


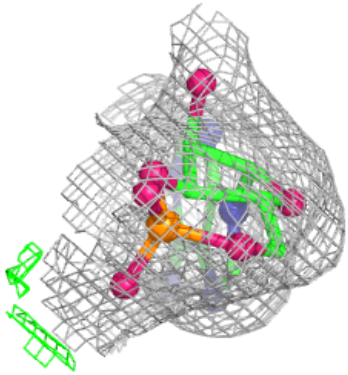


Electron density around CMP J 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

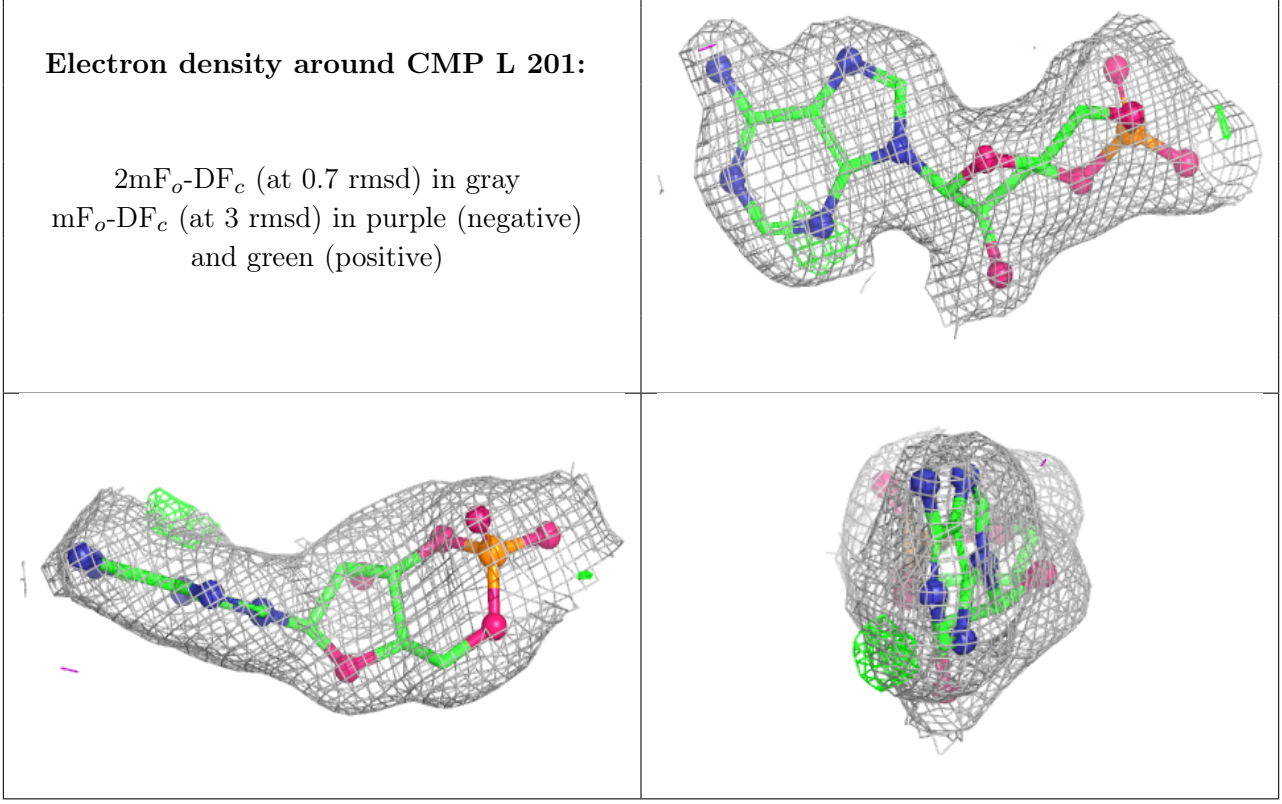






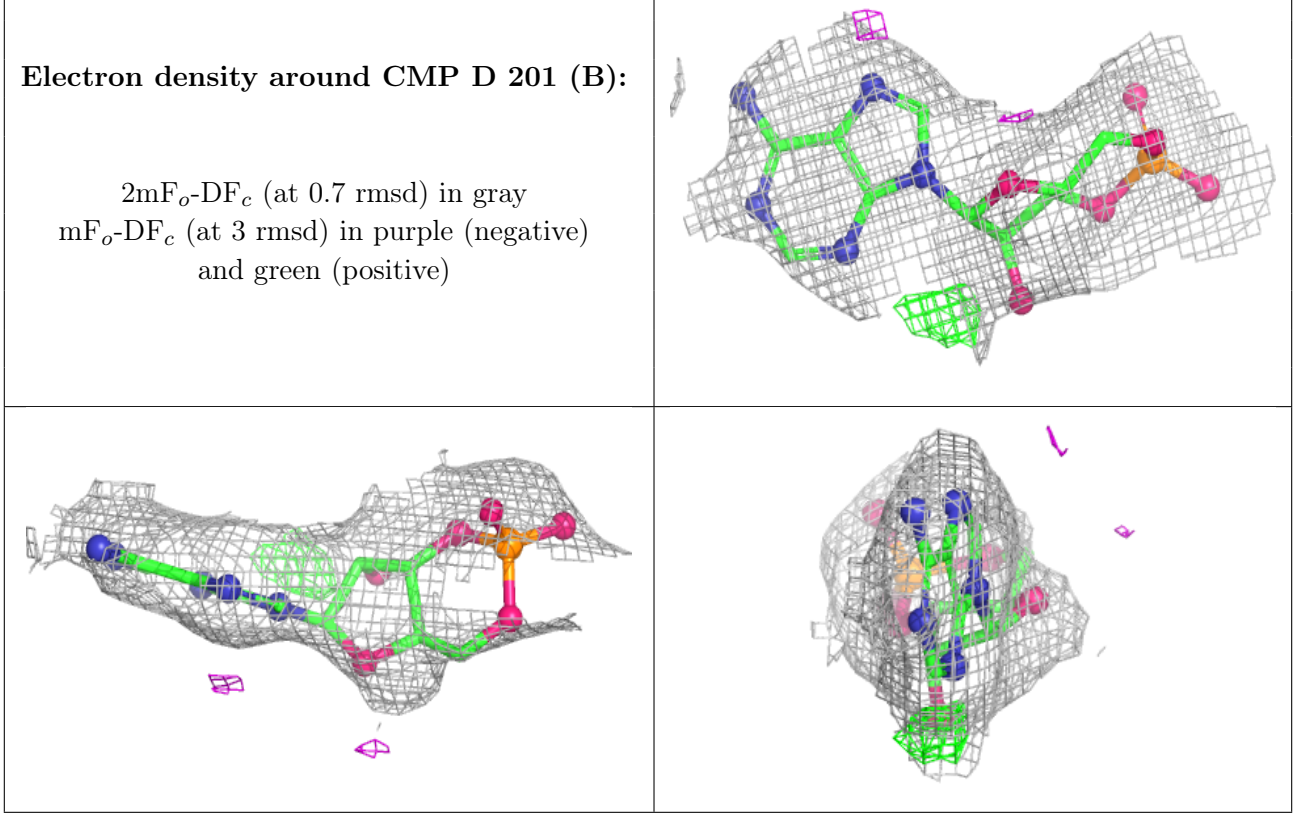
Electron density around CMP L 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



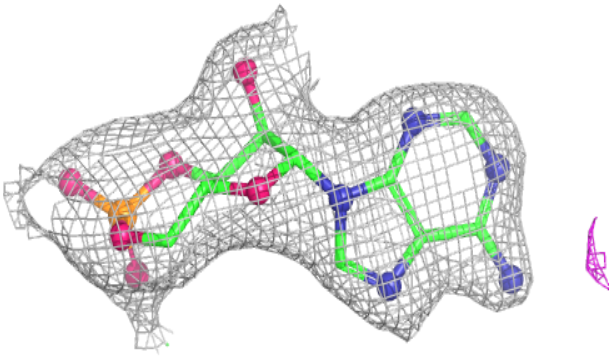
Electron density around CMP D 201 (B):

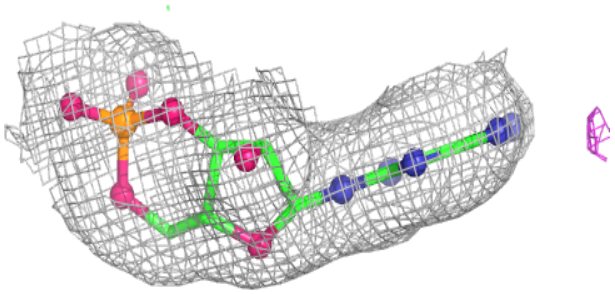
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

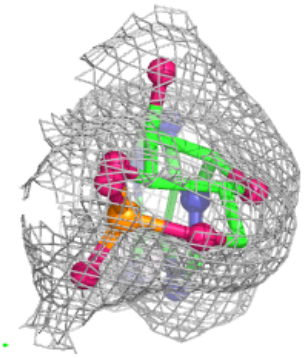


Electron density around CMP E 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

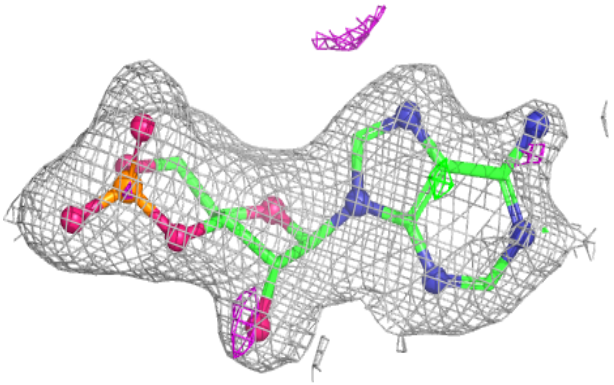


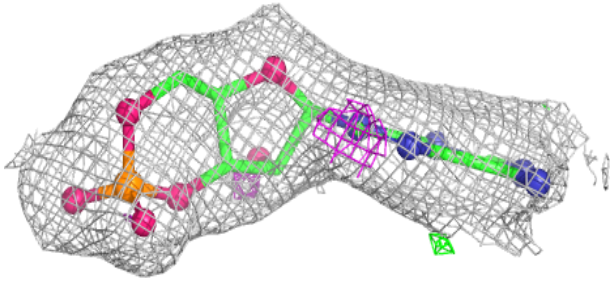


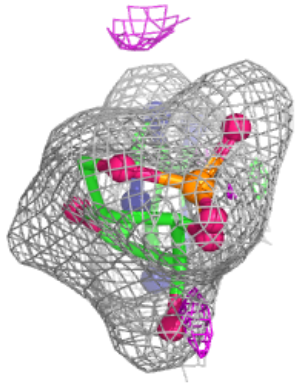


Electron density around CMP B 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

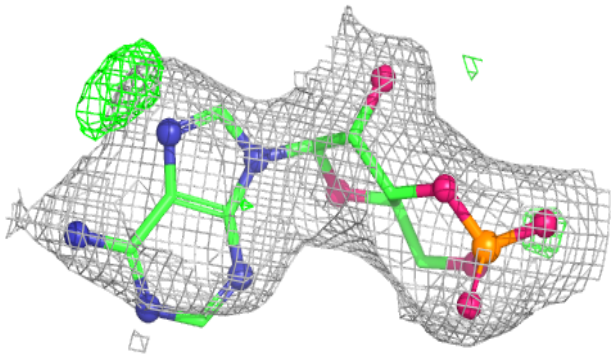


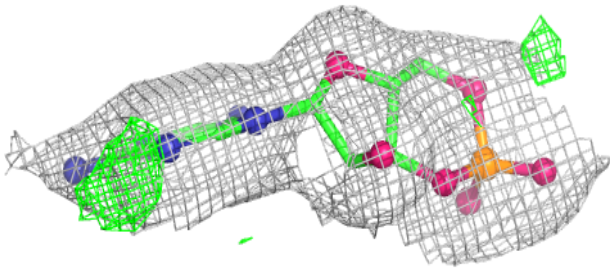


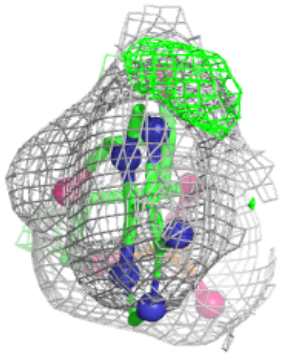


Electron density around CMP B 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

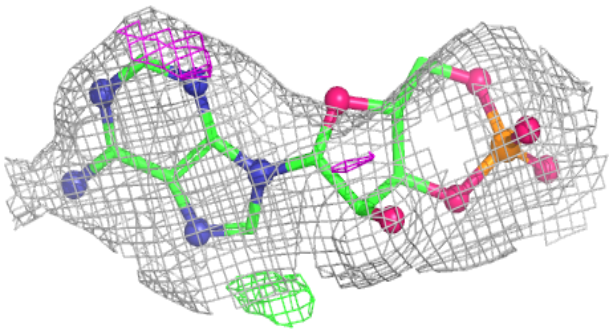


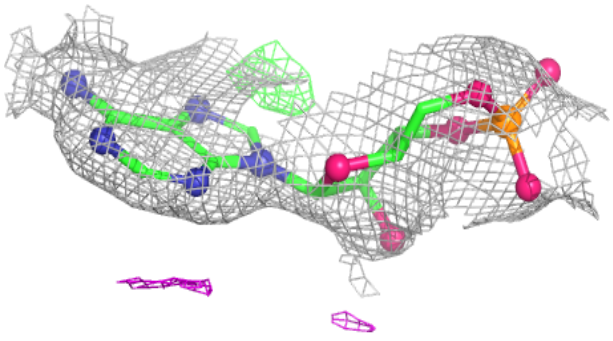


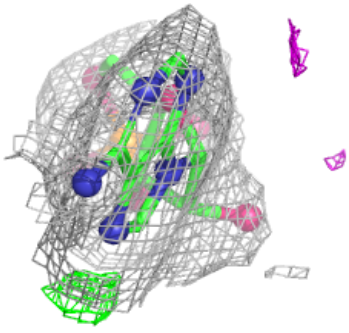


Electron density around CMP D 201 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.